Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:11 PM BST

PDB ID	:	6IWR
Title	:	Crystal structure of GalNAc-T7 with UDP, GalNAc and Mn2+
Authors	:	Yu, C.; Yin, Y.X.
Deposited on	:	2018-12-06
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

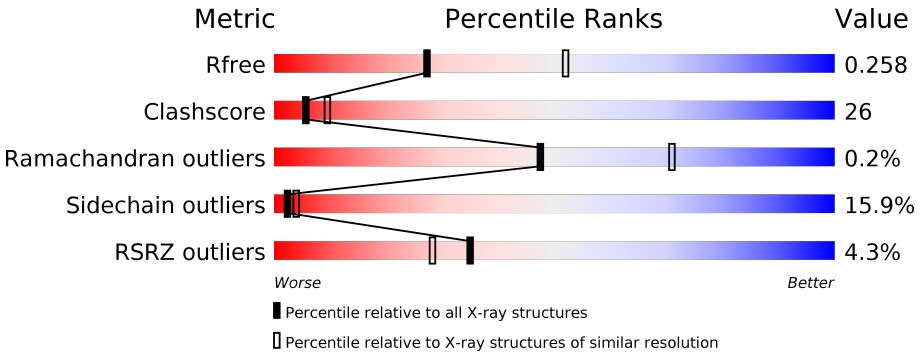
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	597	3% 51% 32% 7% 9%
1	B	597	2% 50% 32% 9% 9%
1	C	597	5% 48% 34% 9% 9%
1	D	597	2% 52% 32% 6% • 10%
1	E	597	5% 53% 31% 7% 9%
1	F	597	7% 53% 32% 7% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27098 atoms, of which 26 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

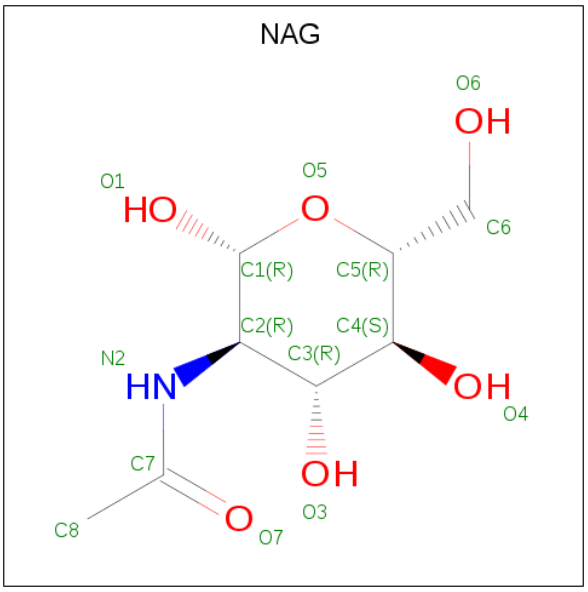
- Molecule 1 is a protein called N-acetylgalactosaminyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	B	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	C	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	D	538	Total	C	N	O	S	0	0	0
			4380	2814	748	795	23			
1	E	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	F	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

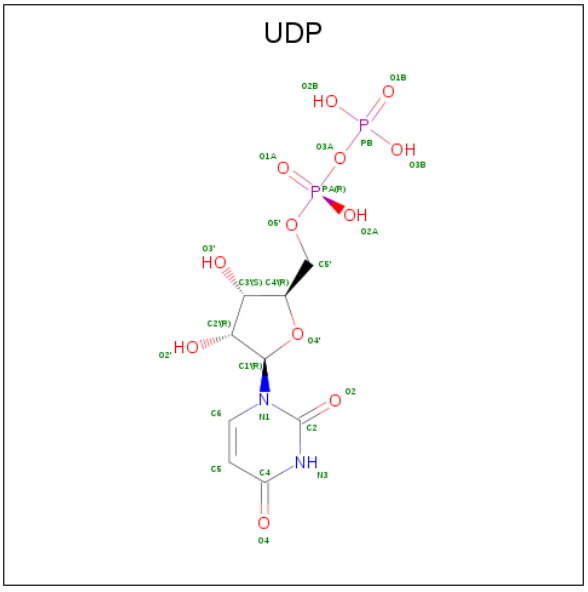
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



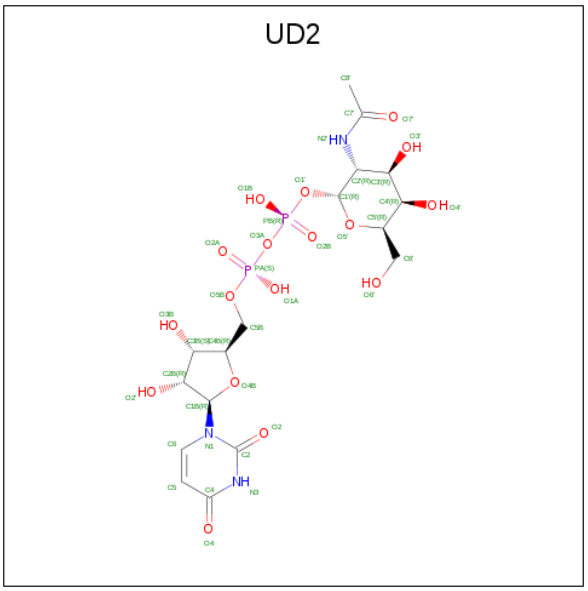
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	H	N	O	0	0
			30	8	15	1	6		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	D	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGALACTOSAMINE (three-letter code: UD2) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 6 is water.

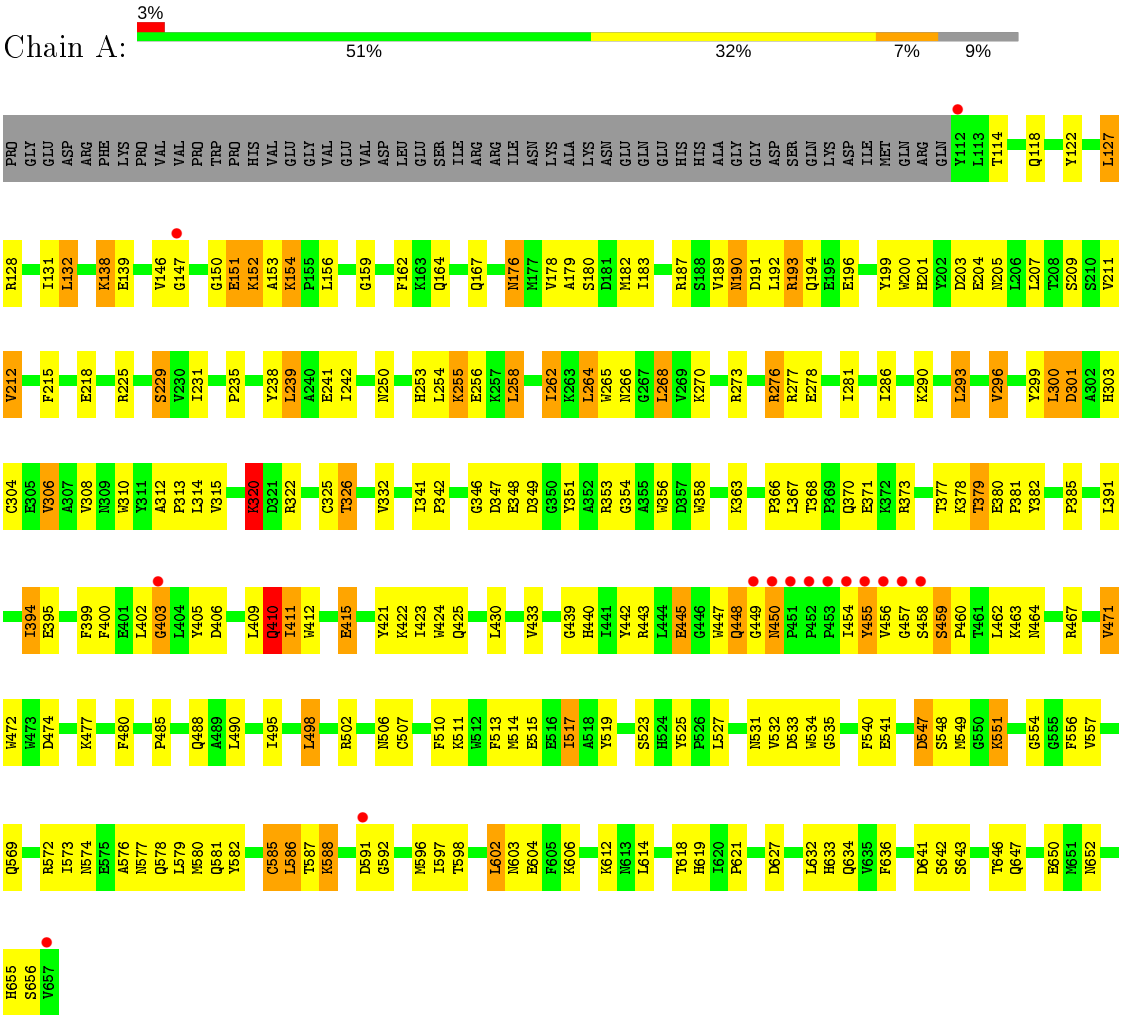
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	100	Total	O	0	0
			100	100		
6	B	77	Total	O	0	0
			77	77		
6	C	60	Total	O	0	0
			60	60		
6	D	55	Total	O	0	0
			55	55		
6	E	68	Total	O	0	0
			68	68		
6	F	47	Total	O	0	0
			47	47		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

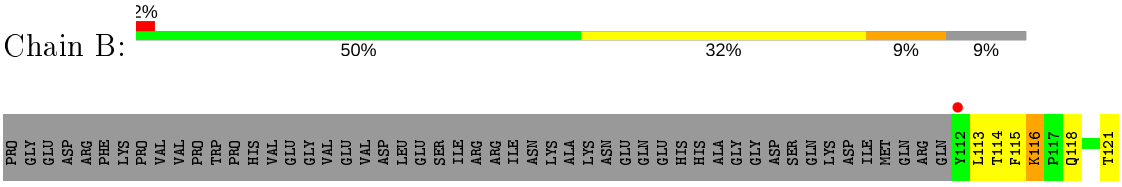
- Molecule 1: N-acetylgalactosaminyltransferase 7

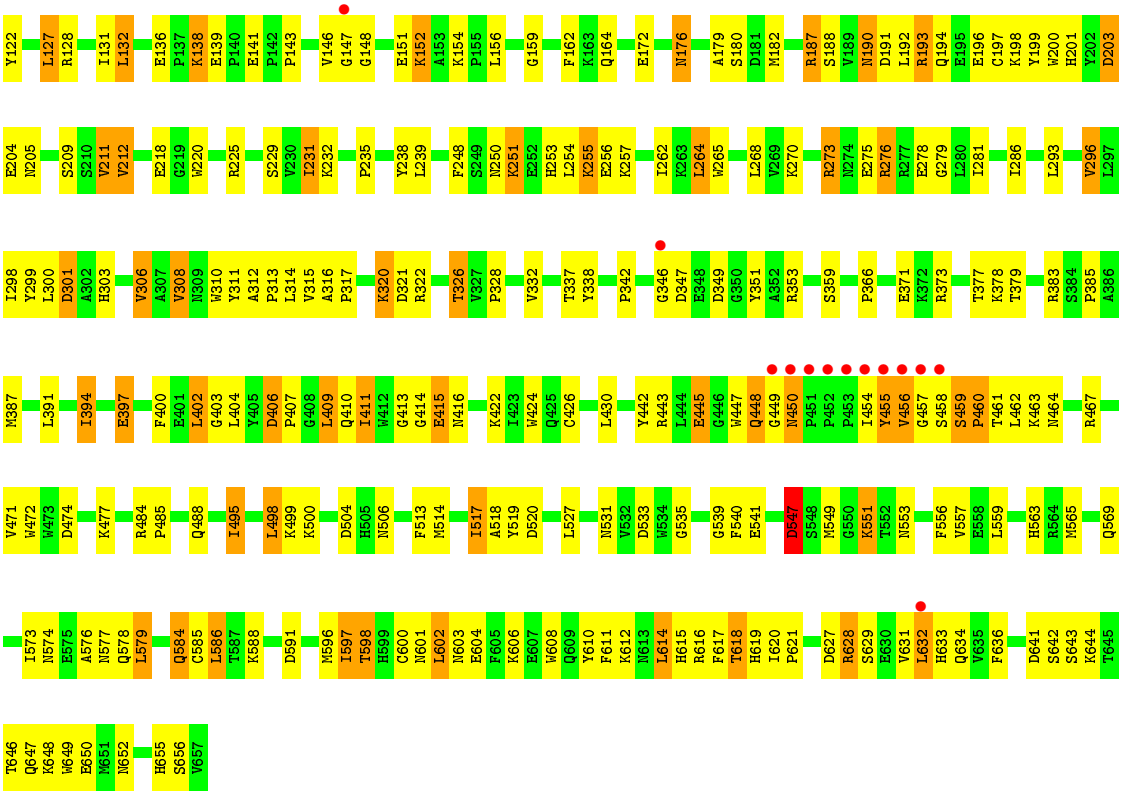
Chain A:



- Molecule 1: N-acetylgalactosaminyltransferase 7

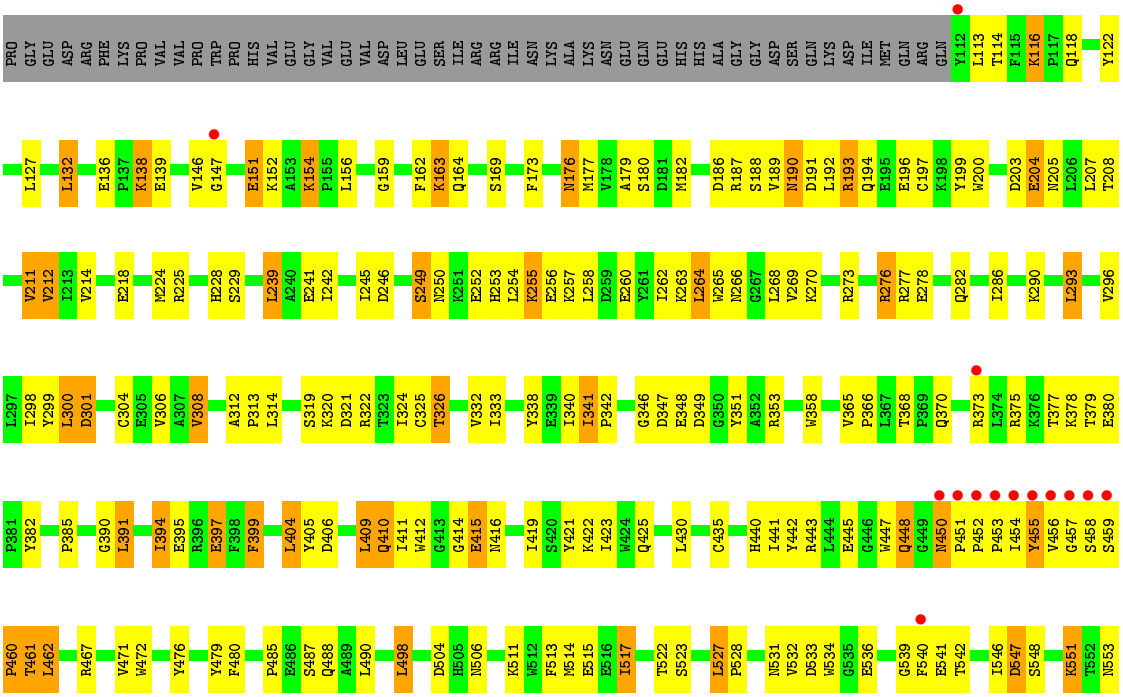
Chain B:

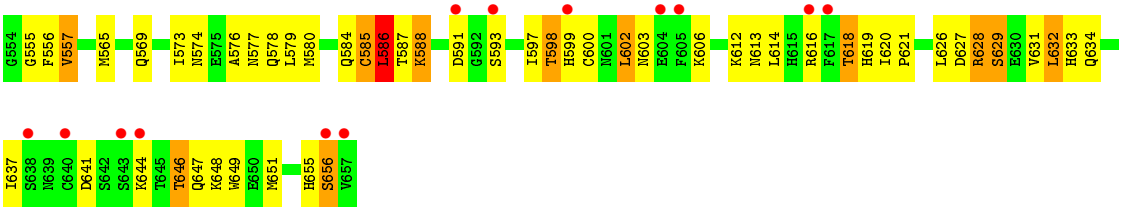




• Molecule 1: N-acetylgalactosaminyltransferase 7

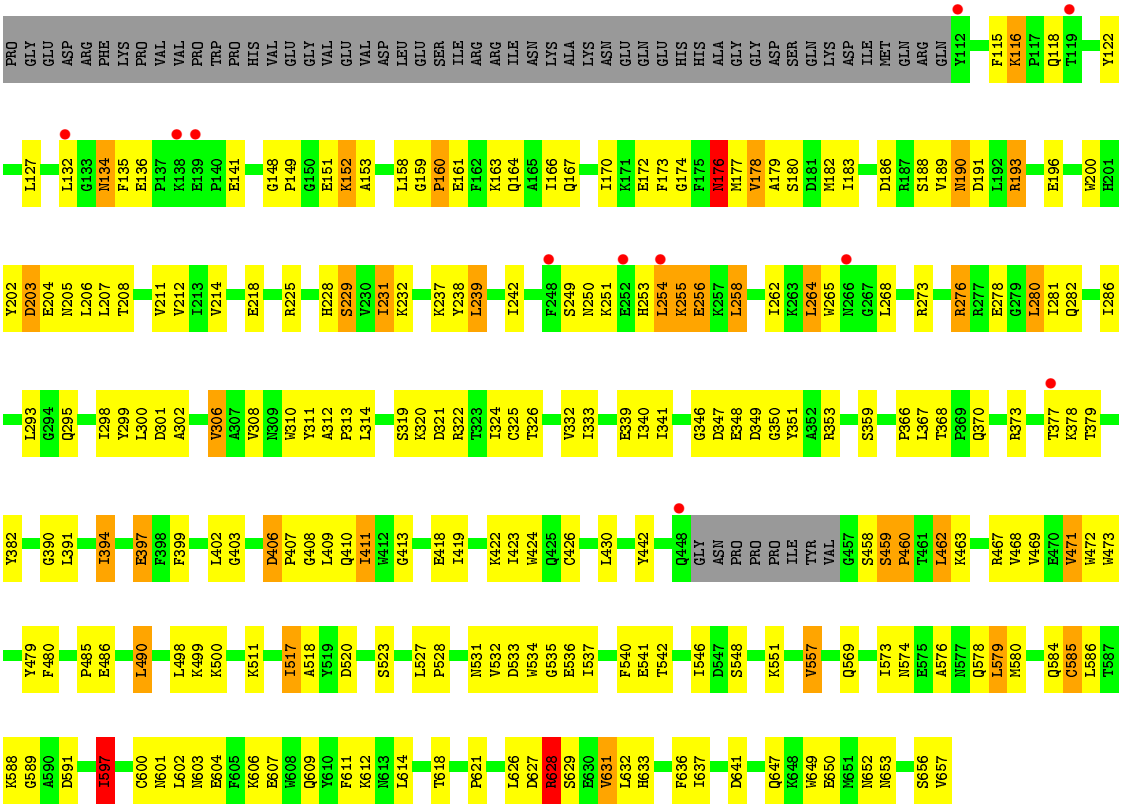
Chain C:





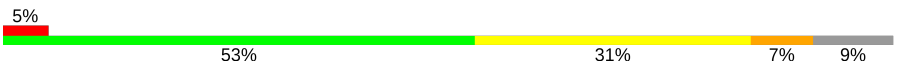
• Molecule 1: N-acetylgalactosaminyltransferase 7

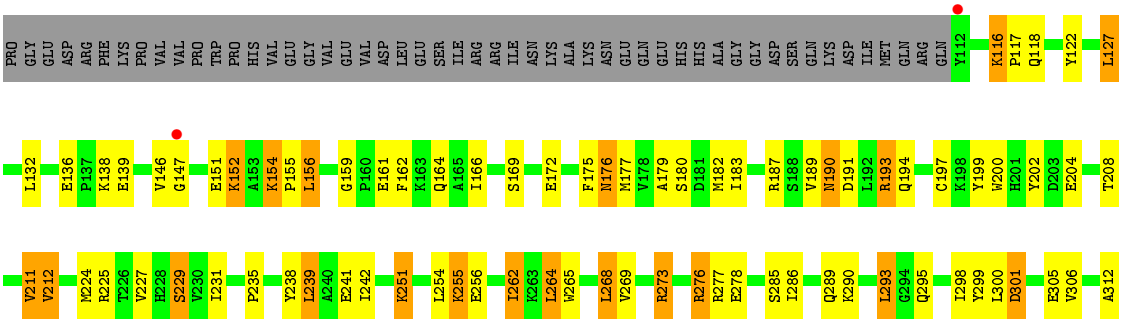
Chain D:

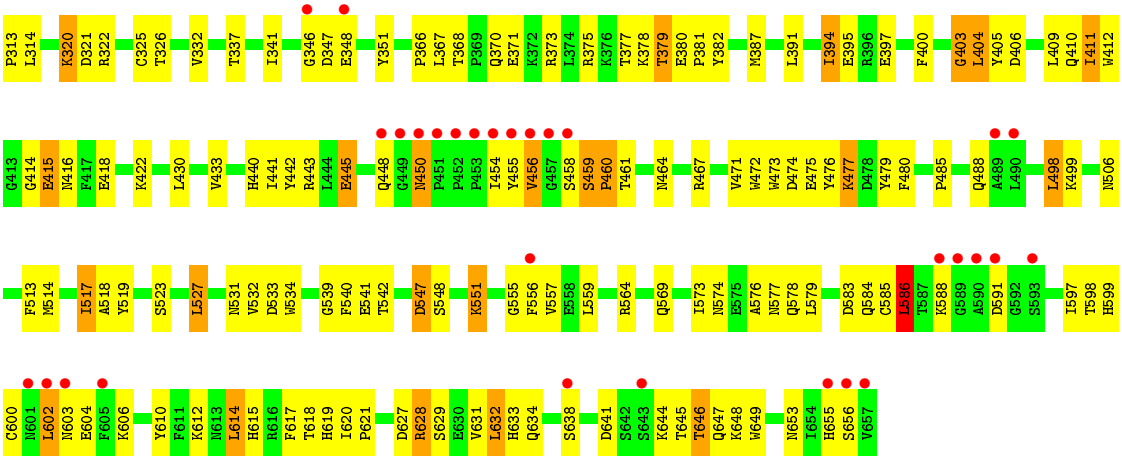


• Molecule 1: N-acetylgalactosaminyltransferase 7

Chain E:

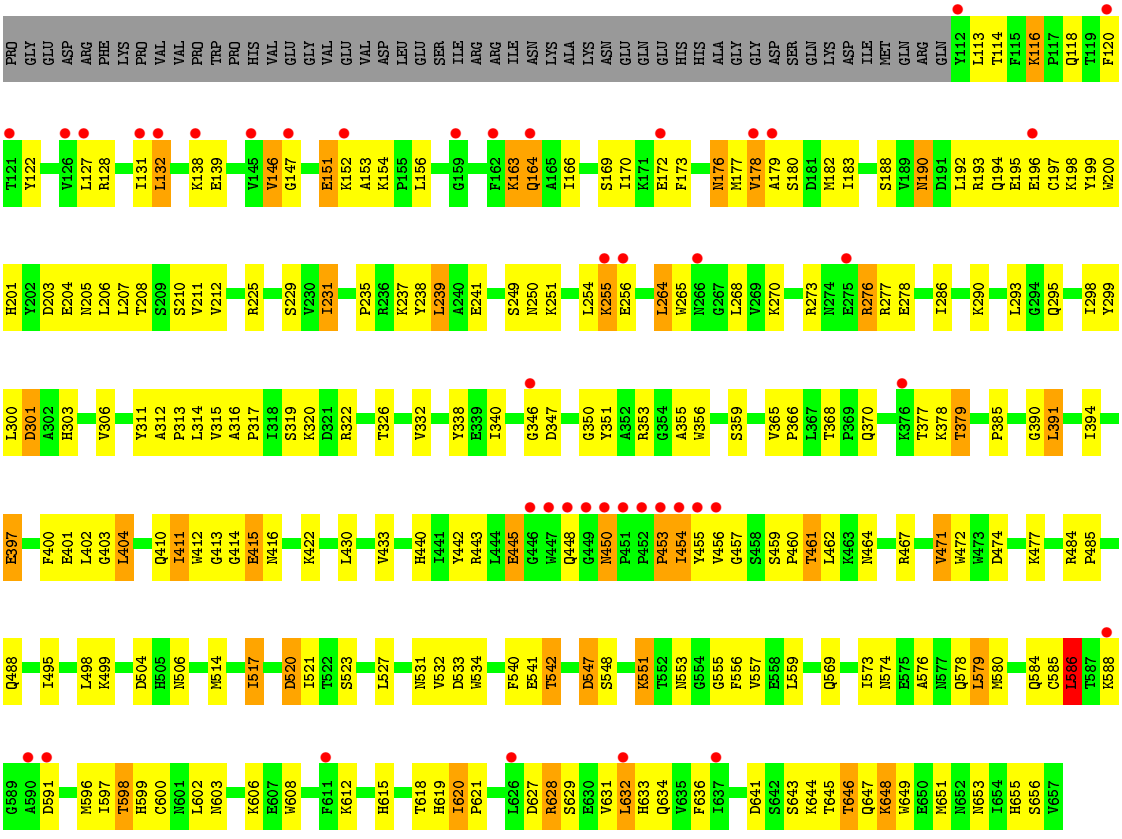






• Molecule 1: N-acetylgalactosaminyltransferase 7

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.44Å 158.26Å 251.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 2.60 49.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.25-2.60) 95.7 (49.25-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.61Å)	Xtriage
Refinement program	PHENIX (dev_2400: ???)	Depositor
R, R_{free}	0.220 , 0.258 0.220 , 0.258	Depositor DCC
R_{free} test set	8025 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	27098	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UD2, UDP, MN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.56	2/4569 (0.0%)	0.71	2/6192 (0.0%)
1	B	0.55	2/4569 (0.0%)	0.70	4/6192 (0.1%)
1	C	0.54	3/4569 (0.1%)	0.68	4/6192 (0.1%)
1	D	0.54	4/4504 (0.1%)	0.70	6/6098 (0.1%)
1	E	0.51	3/4569 (0.1%)	0.66	3/6192 (0.0%)
1	F	0.47	0/4569	0.62	2/6192 (0.0%)
All	All	0.53	14/27349 (0.1%)	0.68	21/37058 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	E	0	1
1	F	0	1
All	All	0	5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	585	CYS	CB-SG	-7.43	1.69	1.82
1	B	585	CYS	CB-SG	-6.53	1.71	1.82
1	D	585	CYS	CB-SG	-5.51	1.72	1.81
1	E	585	CYS	CB-SG	-5.38	1.73	1.81
1	A	320	LYS	CD-CE	5.38	1.64	1.51
1	D	407	PRO	N-CD	5.35	1.55	1.47
1	C	452	PRO	N-CD	5.22	1.55	1.47
1	D	460	PRO	N-CD	5.22	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	117	PRO	N-CD	5.21	1.55	1.47
1	C	585	CYS	CB-SG	-5.21	1.73	1.81
1	D	160	PRO	N-CD	5.15	1.55	1.47
1	B	460	PRO	N-CD	5.10	1.54	1.47
1	C	460	PRO	N-CD	5.09	1.54	1.47
1	E	460	PRO	N-CD	5.06	1.54	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	403	GLY	N-CA-C	8.30	133.84	113.10
1	B	148	GLY	C-N-CD	-7.82	103.39	120.60
1	A	320	LYS	CD-CE-NZ	6.68	127.06	111.70
1	E	403	GLY	N-CA-C	6.63	129.67	113.10
1	B	547	ASP	CB-CG-OD1	6.62	124.26	118.30
1	D	628	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	452	PRO	C-N-CD	6.34	141.72	128.40
1	C	405	TYR	N-CA-C	-6.31	93.97	111.00
1	F	459	SER	C-N-CD	5.95	140.89	128.40
1	C	451	PRO	C-N-CD	5.70	140.36	128.40
1	E	116	LYS	C-N-CD	5.69	140.35	128.40
1	B	459	SER	C-N-CD	5.66	140.28	128.40
1	D	159	GLY	C-N-CD	5.55	140.05	128.40
1	D	459	SER	C-N-CD	5.50	139.95	128.40
1	F	586	LEU	CA-CB-CG	5.48	127.91	115.30
1	D	203	ASP	N-CA-C	-5.35	96.54	111.00
1	C	586	LEU	CA-CB-CG	5.29	127.48	115.30
1	B	320	LYS	CD-CE-NZ	5.26	123.80	111.70
1	A	403	GLY	N-CA-C	5.24	126.21	113.10
1	E	586	LEU	CA-CB-CG	5.18	127.22	115.30
1	D	597	ILE	CG1-CB-CG2	-5.08	100.22	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	GLN	Peptide
1	B	402	LEU	Peptide
1	B	413	GLY	Peptide
1	E	403	GLY	Peptide
1	F	402	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4440	0	4325	212	0
1	B	4440	0	4325	254	0
1	C	4440	0	4325	244	0
1	D	4380	0	4265	228	0
1	E	4440	0	4325	200	0
1	F	4440	0	4325	227	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	D	15	15	15	1	0
4	D	25	11	11	2	0
5	D	39	0	25	3	0
6	A	100	0	0	8	0
6	B	77	0	0	6	0
6	C	60	0	0	1	0
6	D	55	0	0	10	0
6	E	68	0	0	1	0
6	F	47	0	0	4	0
All	All	27072	26	25941	1346	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (1346) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:VAL:HG23	1:B:458:SER:CA	1.41	1.47
1:F:453:PRO:HB2	1:F:455:TYR:CZ	1.56	1.37
1:F:453:PRO:HB2	1:F:455:TYR:CE2	1.62	1.34
1:B:454:ILE:HG22	1:B:457:GLY:CA	1.62	1.27
1:C:454:ILE:O	1:C:458:SER:HA	1.39	1.22
1:B:456:VAL:CG2	1:B:458:SER:HA	1.71	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:GLY:HA2	6:B:821:HOH:O	1.44	1.17
1:F:414:GLY:HA2	1:F:415:GLU:HB3	1.25	1.17
1:F:453:PRO:CB	1:F:455:TYR:CZ	2.26	1.16
1:C:379:THR:CG2	1:C:435:CYS:SG	2.33	1.15
1:A:281:ILE:HG12	1:A:415:GLU:HG2	1.18	1.14
1:B:456:VAL:CG2	1:B:458:SER:CA	2.24	1.14
1:E:564:ARG:HD3	6:E:849:HOH:O	1.46	1.13
1:E:414:GLY:HA2	1:E:415:GLU:HB3	1.28	1.10
1:E:346:GLY:HA3	1:E:366:PRO:HB3	1.31	1.10
1:B:458:SER:HB2	1:B:463:LYS:HD2	1.21	1.09
1:B:454:ILE:HG22	1:B:457:GLY:HA3	1.22	1.09
1:D:347:ASP:HB3	1:D:351:TYR:H	1.12	1.09
1:B:414:GLY:HA2	1:B:415:GLU:HB3	1.35	1.07
1:F:453:PRO:CB	1:F:455:TYR:CE2	2.37	1.07
1:A:455:TYR:HB2	1:A:456:VAL:HG22	1.35	1.06
1:B:454:ILE:CG2	1:B:457:GLY:HA3	1.83	1.06
1:B:456:VAL:HG23	1:B:458:SER:HA	1.23	1.05
1:C:547:ASP:HB2	1:C:569:GLN:HG2	1.39	1.04
1:C:379:THR:HG23	1:C:435:CYS:SG	1.95	1.04
1:B:456:VAL:HG23	1:B:458:SER:N	1.71	1.04
1:B:454:ILE:HG22	1:B:457:GLY:HA2	1.39	1.04
1:B:455:TYR:C	1:B:457:GLY:HA2	1.78	1.04
1:E:456:VAL:HG12	1:E:458:SER:HB3	1.38	1.03
1:C:191:ASP:OD1	1:C:193:ARG:HG2	1.57	1.02
1:D:161:GLU:N	1:D:161:GLU:OE2	1.92	1.02
1:D:579:LEU:HD13	1:D:586:LEU:HD12	1.39	1.02
1:E:456:VAL:HG12	1:E:458:SER:CB	1.88	1.02
1:C:414:GLY:HA2	1:C:415:GLU:HB3	1.37	1.02
1:A:455:TYR:HB2	1:A:456:VAL:CG2	1.90	1.01
1:D:411:ILE:HD11	1:D:460:PRO:HG3	1.43	1.00
1:B:584:GLN:HG3	1:B:598:THR:O	1.61	1.00
1:F:547:ASP:HB2	1:F:569:GLN:HG2	1.36	1.00
1:A:547:ASP:HB2	1:A:569:GLN:HG2	1.41	0.99
1:A:346:GLY:HA3	1:A:366:PRO:HB3	1.41	0.99
1:C:163:LYS:HE3	5:D:704:UD2:O2A	1.63	0.99
1:B:456:VAL:N	1:B:457:GLY:O	1.97	0.98
1:B:346:GLY:HA3	1:B:366:PRO:HB3	1.44	0.97
1:B:456:VAL:N	1:B:457:GLY:C	2.18	0.97
1:A:377:THR:HG22	1:A:379:THR:H	1.29	0.96
1:E:641:ASP:H	1:E:647:GLN:HE22	1.12	0.96
1:B:456:VAL:HG23	1:B:458:SER:C	1.83	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:547:ASP:HB2	1:E:569:GLN:HG2	1.46	0.96
1:B:514:MET:HA	1:B:514:MET:HE2	1.48	0.96
1:C:346:GLY:HA3	1:C:366:PRO:HB3	1.49	0.95
1:B:456:VAL:HG21	1:B:458:SER:O	1.66	0.94
1:B:458:SER:CB	1:B:463:LYS:HD2	1.97	0.94
1:B:547:ASP:HB2	1:B:569:GLN:HG2	1.45	0.94
1:F:641:ASP:H	1:F:647:GLN:HE22	0.97	0.94
1:B:458:SER:H	1:B:459:SER:HA	1.29	0.94
1:B:132:LEU:HD23	1:B:199:TYR:HE1	1.32	0.94
1:C:411:ILE:HD12	1:C:412:TRP:N	1.81	0.94
1:F:410:GLN:H	1:F:464:ASN:HD21	1.06	0.94
1:B:458:SER:HB2	1:B:463:LYS:CD	1.98	0.93
1:C:632:LEU:CD1	1:C:634:GLN:HB2	1.98	0.93
1:B:132:LEU:HD23	1:B:199:TYR:CE1	2.03	0.93
1:E:404:LEU:HD22	1:E:404:LEU:H	1.28	0.93
1:F:453:PRO:HG2	1:F:455:TYR:HE2	1.33	0.93
1:C:641:ASP:H	1:C:647:GLN:HE22	1.07	0.92
1:A:341:ILE:CG2	1:B:632:LEU:HB2	2.00	0.92
1:C:282:GLN:HG3	1:C:410:GLN:NE2	1.85	0.91
1:B:132:LEU:CD2	1:B:199:TYR:CE1	2.53	0.91
1:C:462:LEU:HD11	1:C:487:SER:HB3	1.52	0.91
1:E:632:LEU:CD1	1:E:634:GLN:HB2	2.00	0.91
1:A:281:ILE:CG1	1:A:415:GLU:HG2	2.00	0.90
1:B:456:VAL:CG2	1:B:458:SER:C	2.40	0.90
1:F:193:ARG:HD2	1:F:197:CYS:SG	2.11	0.90
1:C:412:TRP:O	1:C:461:THR:HG22	1.71	0.90
1:F:414:GLY:HA2	1:F:415:GLU:CB	2.01	0.90
1:D:631:VAL:HG22	1:D:632:LEU:HD12	1.52	0.89
1:F:377:THR:HG22	1:F:379:THR:H	1.38	0.89
1:E:414:GLY:HA2	1:E:415:GLU:CB	2.01	0.89
1:B:641:ASP:H	1:B:647:GLN:HE22	1.17	0.89
1:B:414:GLY:HA2	1:B:415:GLU:CB	1.99	0.89
1:C:151:GLU:HA	1:C:152:LYS:O	1.71	0.89
1:C:454:ILE:O	1:C:458:SER:CA	2.21	0.89
1:A:422:LYS:HG2	1:A:472:TRP:CZ2	2.08	0.88
1:F:347:ASP:HB3	1:F:351:TYR:H	1.35	0.88
1:F:453:PRO:HG2	1:F:455:TYR:CE2	2.08	0.88
1:A:276:ARG:HD2	1:A:278:GLU:OE2	1.73	0.88
1:A:641:ASP:H	1:A:647:GLN:HE22	1.16	0.88
1:C:467:ARG:O	1:C:471:VAL:HG12	1.73	0.88
1:F:453:PRO:CG	1:F:455:TYR:CE2	2.57	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:455:TYR:HB2	1:E:456:VAL:HG22	1.55	0.87
1:B:377:THR:HG22	1:B:379:THR:H	1.37	0.87
1:B:458:SER:CB	1:B:463:LYS:CD	2.53	0.86
1:D:163:LYS:O	1:D:167:GLN:HG3	1.74	0.86
1:A:485:PRO:O	1:A:488:GLN:HG3	1.75	0.86
1:F:314:LEU:HD12	1:F:326:THR:HG22	1.57	0.86
1:B:467:ARG:O	1:B:471:VAL:HG12	1.76	0.86
1:C:163:LYS:CE	5:D:704:UD2:O2A	2.23	0.86
1:E:414:GLY:HA3	1:E:416:ASN:H	1.40	0.86
1:E:619:HIS:CE1	1:E:621:PRO:HG2	2.11	0.86
1:A:511:LYS:HE3	1:A:515:GLU:OE2	1.77	0.85
1:E:346:GLY:CA	1:E:366:PRO:HB3	2.07	0.85
1:E:459:SER:OG	1:E:460:PRO:CD	2.24	0.85
1:E:346:GLY:HA3	1:E:366:PRO:CB	2.04	0.85
1:A:458:SER:OG	1:A:462:LEU:HB2	1.75	0.84
1:A:458:SER:OG	1:A:462:LEU:CB	2.26	0.84
1:D:251:LYS:HB3	1:D:253:HIS:CD2	2.11	0.84
1:F:632:LEU:CD1	1:F:634:GLN:HB2	2.08	0.84
1:B:458:SER:OG	1:B:463:LYS:HG3	1.76	0.84
1:D:160:PRO:HA	1:D:163:LYS:HE3	1.58	0.84
1:C:118:GLN:HE22	1:C:322:ARG:H	1.25	0.84
1:D:347:ASP:HB3	1:D:351:TYR:N	1.93	0.84
1:B:632:LEU:CD1	1:B:634:GLN:HB2	2.09	0.83
1:B:619:HIS:CE1	1:B:621:PRO:HG2	2.13	0.83
1:A:191:ASP:OD1	1:A:193:ARG:HG2	1.76	0.83
1:B:422:LYS:HG2	1:B:472:TRP:CZ2	2.13	0.83
1:E:410:GLN:H	1:E:464:ASN:HD21	1.23	0.83
1:B:458:SER:CB	1:B:463:LYS:HG3	2.09	0.83
1:E:467:ARG:O	1:E:471:VAL:HG12	1.78	0.83
1:A:347:ASP:HB3	1:A:351:TYR:H	1.42	0.83
1:B:132:LEU:CD2	1:B:199:TYR:HE1	1.89	0.82
1:A:281:ILE:HG12	1:A:415:GLU:CG	2.07	0.82
1:C:414:GLY:HA2	1:C:415:GLU:CB	2.09	0.82
1:A:632:LEU:HD23	1:B:342:PRO:HG2	1.61	0.82
1:C:454:ILE:O	1:C:457:GLY:HA3	1.78	0.82
1:D:127:LEU:HD11	1:D:196:GLU:HG2	1.60	0.82
1:B:456:VAL:N	1:B:457:GLY:CA	2.43	0.82
1:E:459:SER:OG	1:E:460:PRO:HD2	1.80	0.81
1:B:347:ASP:HB3	1:B:351:TYR:H	1.46	0.81
1:F:454:ILE:HG23	1:F:457:GLY:CA	2.10	0.81
1:D:348:GLU:N	1:D:348:GLU:OE1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:SER:HB3	1:B:459:SER:O	1.80	0.81
1:C:122:TYR:CE1	1:C:203:ASP:HB3	2.16	0.80
1:C:314:LEU:HD12	1:C:326:THR:CG2	2.12	0.80
1:F:193:ARG:CD	1:F:197:CYS:HB3	2.12	0.80
1:B:632:LEU:HD11	1:B:634:GLN:CD	2.03	0.80
1:B:458:SER:OG	1:B:463:LYS:CG	2.29	0.79
1:D:251:LYS:HB3	1:D:253:HIS:NE2	1.96	0.79
1:F:485:PRO:O	1:F:488:GLN:HG3	1.82	0.79
1:D:347:ASP:HB2	1:D:351:TYR:O	1.82	0.79
1:F:193:ARG:CD	1:F:197:CYS:CB	2.60	0.79
1:E:513:PHE:CE1	1:E:517:ILE:HD11	2.18	0.79
1:F:410:GLN:N	1:F:464:ASN:HD21	1.80	0.79
1:F:619:HIS:CE1	1:F:621:PRO:HG2	2.18	0.79
1:C:196:GLU:OE1	1:C:379:THR:HB	1.83	0.79
1:D:422:LYS:HG2	1:D:472:TRP:CZ2	2.18	0.78
1:B:414:GLY:HA3	1:B:416:ASN:H	1.46	0.78
1:C:632:LEU:HD11	1:C:634:GLN:HB2	1.62	0.78
1:D:641:ASP:H	1:D:647:GLN:HE22	1.29	0.78
1:B:196:GLU:OE2	1:B:377:THR:HG23	1.84	0.78
1:A:347:ASP:HB2	1:A:351:TYR:O	1.83	0.77
1:C:379:THR:HG21	1:C:435:CYS:SG	2.22	0.77
1:F:193:ARG:NE	1:F:197:CYS:HB3	1.99	0.77
1:A:314:LEU:HD12	1:A:326:THR:CG2	2.14	0.77
1:D:609:GLN:HG2	1:D:618:THR:HG23	1.65	0.77
1:F:193:ARG:HD2	1:F:197:CYS:HB3	1.67	0.77
1:F:410:GLN:H	1:F:464:ASN:ND2	1.83	0.77
1:F:193:ARG:HD2	1:F:197:CYS:CB	2.14	0.77
1:C:632:LEU:HD22	1:C:633:HIS:H	1.50	0.76
1:E:632:LEU:C	1:E:632:LEU:HD13	2.06	0.76
1:B:118:GLN:HE22	1:B:322:ARG:H	1.33	0.76
1:A:346:GLY:CA	1:A:366:PRO:HB3	2.15	0.76
1:C:628:ARG:HH11	1:C:628:ARG:HG3	1.50	0.76
1:F:467:ARG:O	1:F:471:VAL:HG12	1.84	0.76
1:D:373:ARG:CZ	6:D:805:HOH:O	2.33	0.76
1:D:628:ARG:HG2	1:D:628:ARG:HH11	1.50	0.76
1:B:485:PRO:O	1:B:488:GLN:HG3	1.85	0.76
1:D:411:ILE:CD1	1:D:460:PRO:HG3	2.16	0.76
1:A:346:GLY:HA3	1:A:366:PRO:CB	2.16	0.76
1:D:251:LYS:CB	1:D:253:HIS:NE2	2.49	0.76
1:B:347:ASP:HB2	1:B:351:TYR:O	1.84	0.75
1:B:456:VAL:CG2	1:B:458:SER:O	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:LEU:N	1:B:586:LEU:HD23	2.01	0.75
1:C:122:TYR:CZ	1:C:203:ASP:HB3	2.19	0.75
1:C:377:THR:HG22	1:C:379:THR:H	1.51	0.75
1:C:619:HIS:CE1	1:C:621:PRO:HG2	2.21	0.75
1:F:414:GLY:HA3	1:F:416:ASN:OD1	1.86	0.75
1:B:458:SER:CB	1:B:463:LYS:CG	2.65	0.75
1:E:414:GLY:CA	1:E:416:ASN:H	2.00	0.75
1:E:414:GLY:CA	1:E:415:GLU:HB3	2.14	0.75
1:F:347:ASP:HB3	1:F:351:TYR:N	2.02	0.75
1:F:628:ARG:HD2	1:F:646:THR:HG22	1.69	0.75
1:B:632:LEU:C	1:B:632:LEU:HD13	2.07	0.75
1:C:632:LEU:C	1:C:632:LEU:HD13	2.06	0.75
1:D:158:LEU:CD1	1:D:178:VAL:CG2	2.65	0.75
1:F:193:ARG:CG	1:F:197:CYS:SG	2.75	0.74
1:F:314:LEU:HD12	1:F:326:THR:CG2	2.17	0.74
1:A:314:LEU:CD1	1:A:326:THR:HG22	2.17	0.74
1:B:414:GLY:HA3	1:B:416:ASN:OD1	1.88	0.74
1:D:314:LEU:O	1:D:326:THR:HG21	1.87	0.74
1:F:574:ASN:HB3	1:F:576:ALA:H	1.53	0.74
1:F:632:LEU:HD12	6:F:807:HOH:O	1.86	0.74
1:A:467:ARG:O	1:A:471:VAL:HG12	1.87	0.74
1:D:471:VAL:HG22	1:D:472:TRP:CD1	2.23	0.73
1:A:547:ASP:HB2	1:A:569:GLN:CG	2.17	0.73
1:B:455:TYR:C	1:B:457:GLY:CA	2.55	0.73
1:E:422:LYS:HG2	1:E:472:TRP:CZ2	2.24	0.73
1:C:632:LEU:HB2	1:D:341:ILE:CG2	2.19	0.73
1:F:151:GLU:HA	1:F:152:LYS:C	2.09	0.73
1:C:347:ASP:HB3	1:C:351:TYR:H	1.53	0.72
1:F:411:ILE:HG22	1:F:412:TRP:N	2.03	0.72
1:A:349:ASP:CG	6:A:810:HOH:O	2.26	0.72
1:E:628:ARG:HD2	1:E:646:THR:HG22	1.69	0.72
1:D:160:PRO:HA	1:D:163:LYS:HG3	1.71	0.72
1:D:122:TYR:CZ	1:D:203:ASP:HB3	2.25	0.72
1:C:414:GLY:HA3	1:C:416:ASN:OD1	1.88	0.72
1:B:584:GLN:HG2	1:B:597:ILE:HG23	1.70	0.72
1:A:196:GLU:OE2	1:A:377:THR:HG23	1.89	0.72
1:A:547:ASP:CB	1:A:569:GLN:HG2	2.18	0.72
1:C:191:ASP:OD1	1:C:193:ARG:CG	2.38	0.72
1:E:224:MET:HE3	1:E:224:MET:HA	1.71	0.72
1:D:200:TRP:HZ2	1:D:377:THR:HG21	1.55	0.71
1:B:455:TYR:CA	1:B:457:GLY:HA2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ASP:OD2	1:C:205:ASN:HB2	1.90	0.71
1:C:540:PHE:O	1:C:542:THR:HG23	1.89	0.71
1:C:632:LEU:HB2	1:D:341:ILE:HG22	1.72	0.71
1:D:314:LEU:CD1	1:D:326:THR:HG22	2.20	0.71
1:D:118:GLN:NE2	1:D:322:ARG:H	1.87	0.71
1:B:191:ASP:OD1	1:B:193:ARG:HG2	1.91	0.71
1:C:136:GLU:OE1	1:C:193:ARG:NH2	2.21	0.71
1:F:332:VAL:HG13	1:F:442:TYR:HD2	1.55	0.71
1:E:632:LEU:HD13	1:E:634:GLN:HB2	1.73	0.71
1:D:207:LEU:HD13	1:D:319:SER:OG	1.89	0.71
1:F:414:GLY:CA	1:F:415:GLU:HB3	2.12	0.71
1:E:377:THR:HG22	1:E:379:THR:H	1.56	0.70
1:F:193:ARG:CD	1:F:197:CYS:SG	2.79	0.70
1:F:314:LEU:CD1	1:F:326:THR:HG22	2.20	0.70
1:C:513:PHE:CE1	1:C:517:ILE:HD11	2.26	0.70
1:D:580:MET:HG2	1:D:585:CYS:SG	2.32	0.70
1:E:406:ASP:OD1	1:E:498:LEU:HD11	1.91	0.70
1:A:574:ASN:HB3	1:A:576:ALA:H	1.55	0.70
1:F:453:PRO:CB	1:F:455:TYR:OH	2.38	0.70
1:D:629:SER:OG	1:D:632:LEU:HD13	1.91	0.70
1:A:194:GLN:HE22	1:A:349:ASP:CG	1.95	0.70
1:B:514:MET:HE2	1:B:518:ALA:HB3	1.74	0.70
1:C:399:PHE:CE1	1:C:404:LEU:O	2.45	0.70
1:C:314:LEU:CD1	1:C:326:THR:CG2	2.70	0.69
1:F:347:ASP:HB2	1:F:351:TYR:O	1.92	0.69
1:A:459:SER:HB3	1:A:460:PRO:CD	2.23	0.69
1:E:314:LEU:CD1	1:E:326:THR:HG22	2.22	0.69
1:A:332:VAL:HG13	1:A:442:TYR:HD2	1.56	0.69
1:B:450:ASN:N	1:B:450:ASN:HD22	1.89	0.69
1:C:118:GLN:NE2	1:C:322:ARG:H	1.90	0.69
1:E:628:ARG:HH11	1:E:628:ARG:HG3	1.58	0.69
1:C:632:LEU:HD13	1:C:634:GLN:HB2	1.75	0.69
1:D:332:VAL:HG13	1:D:442:TYR:CD2	2.28	0.69
1:D:141:GLU:OE1	1:D:232:LYS:NZ	2.22	0.69
1:F:422:LYS:HG2	1:F:472:TRP:CZ2	2.27	0.69
1:B:203:ASP:OD2	1:B:205:ASN:HB2	1.93	0.69
1:A:457:GLY:C	1:A:459:SER:HB2	2.12	0.68
1:C:450:ASN:HD22	1:C:450:ASN:N	1.91	0.68
1:F:122:TYR:CZ	1:F:203:ASP:HB3	2.28	0.68
1:F:454:ILE:HG23	1:F:457:GLY:N	2.08	0.68
1:C:602:LEU:HD22	1:C:602:LEU:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:ILE:HD11	1:D:460:PRO:CG	2.23	0.68
1:E:456:VAL:HG12	1:E:458:SER:OG	1.93	0.68
1:A:132:LEU:HD23	1:A:199:TYR:CE1	2.29	0.68
1:A:458:SER:N	1:A:459:SER:HA	2.06	0.68
1:E:347:ASP:HB2	1:E:351:TYR:O	1.92	0.68
1:B:414:GLY:CA	1:B:416:ASN:H	2.07	0.68
1:F:193:ARG:HE	1:F:197:CYS:HB3	1.57	0.68
1:C:314:LEU:CD1	1:C:326:THR:HG22	2.24	0.68
1:D:314:LEU:HD12	1:D:326:THR:CG2	2.23	0.68
1:E:471:VAL:HG13	1:E:472:TRP:CD1	2.28	0.68
1:B:346:GLY:HA3	1:B:366:PRO:CB	2.23	0.68
1:D:208:THR:OG1	1:D:295:GLN:HG3	1.94	0.68
1:B:458:SER:HB3	1:B:459:SER:C	2.15	0.68
1:F:540:PHE:CD2	1:F:541:GLU:HG3	2.29	0.68
1:A:286:ILE:CG2	1:A:290:LYS:HD2	2.24	0.68
1:B:212:VAL:HG21	1:B:299:TYR:CE1	2.28	0.68
1:F:203:ASP:O	1:F:204:GLU:HB2	1.92	0.68
1:F:411:ILE:HG22	1:F:412:TRP:H	1.56	0.68
1:C:565:MET:HE2	1:D:163:LYS:HZ1	1.58	0.67
1:A:450:ASN:N	1:A:450:ASN:HD22	1.92	0.67
1:D:255:LYS:C	1:D:256:GLU:HG2	2.13	0.67
1:D:390:GLY:C	1:D:391:LEU:HD23	2.14	0.67
1:C:282:GLN:NE2	1:C:409:LEU:O	2.24	0.67
1:E:450:ASN:HD22	1:E:450:ASN:N	1.92	0.67
1:F:632:LEU:C	1:F:632:LEU:HD13	2.15	0.67
1:B:346:GLY:CA	1:B:366:PRO:HB3	2.23	0.67
1:F:574:ASN:HB3	1:F:576:ALA:N	2.09	0.67
1:F:628:ARG:HH11	1:F:628:ARG:HG3	1.60	0.67
1:C:347:ASP:HB2	1:C:351:TYR:O	1.94	0.67
1:C:422:LYS:HG2	1:C:472:TRP:CZ2	2.30	0.67
1:C:641:ASP:HB3	1:C:644:LYS:HG3	1.76	0.67
1:E:314:LEU:HD12	1:E:326:THR:CG2	2.23	0.66
1:D:164:GLN:HA	1:D:164:GLN:OE1	1.94	0.66
1:E:632:LEU:HD11	1:E:634:GLN:HB2	1.76	0.66
1:D:200:TRP:CZ2	1:D:377:THR:HG21	2.29	0.66
1:B:414:GLY:CA	1:B:415:GLU:HB3	2.21	0.66
1:B:547:ASP:HB2	1:B:569:GLN:CG	2.21	0.66
1:C:346:GLY:HA3	1:C:366:PRO:CB	2.22	0.66
1:B:559:LEU:O	1:B:633:HIS:HB3	1.96	0.66
1:C:586:LEU:HD23	1:C:586:LEU:N	2.10	0.66
1:E:314:LEU:O	1:E:326:THR:HG21	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:SER:N	1:B:459:SER:HA	2.06	0.66
1:C:118:GLN:HE22	1:C:322:ARG:N	1.94	0.66
1:D:251:LYS:CB	1:D:253:HIS:CD2	2.79	0.66
1:D:333:ILE:HG12	1:D:340:ILE:HG12	1.77	0.66
1:E:632:LEU:HD22	1:E:633:HIS:H	1.60	0.66
1:F:122:TYR:CE2	1:F:203:ASP:HB3	2.31	0.66
1:B:514:MET:CE	1:B:518:ALA:HB3	2.26	0.65
1:C:632:LEU:HD22	1:C:633:HIS:N	2.10	0.65
1:E:410:GLN:N	1:E:464:ASN:HD21	1.94	0.65
1:E:574:ASN:HB2	1:E:578:GLN:H	1.61	0.65
1:F:632:LEU:HD11	1:F:634:GLN:CD	2.16	0.65
1:C:325:CYS:HB2	1:C:394:ILE:HG23	1.77	0.65
1:C:574:ASN:HB3	1:C:576:ALA:H	1.60	0.65
1:D:158:LEU:CD1	1:D:178:VAL:HG23	2.27	0.65
1:E:627:ASP:OD1	1:E:646:THR:HB	1.95	0.65
1:C:511:LYS:HE3	1:C:515:GLU:OE2	1.97	0.65
1:D:179:ALA:O	1:D:183:ILE:HG13	1.97	0.65
1:A:354:GLY:O	1:A:385:PRO:HD2	1.97	0.65
1:B:458:SER:H	1:B:459:SER:CA	2.05	0.65
1:D:467:ARG:O	1:D:471:VAL:HG13	1.97	0.65
1:E:547:ASP:HB2	1:E:569:GLN:CG	2.24	0.65
1:F:632:LEU:HD13	1:F:634:GLN:HB2	1.77	0.65
1:D:135:PHE:CE2	1:D:202:TYR:HB2	2.32	0.65
1:E:211:VAL:HG22	1:E:242:ILE:HG12	1.79	0.65
1:B:118:GLN:NE2	1:B:322:ARG:H	1.95	0.64
1:F:414:GLY:HA3	1:F:416:ASN:H	1.61	0.64
1:A:373:ARG:O	1:A:373:ARG:HD2	1.97	0.64
1:A:255:LYS:O	1:A:256:GLU:HB2	1.96	0.64
1:E:276:ARG:HD2	1:E:278:GLU:OE2	1.98	0.64
1:E:586:LEU:HD23	1:E:586:LEU:N	2.12	0.64
1:F:450:ASN:N	1:F:450:ASN:HD22	1.94	0.64
1:A:458:SER:OG	1:A:462:LEU:HB3	1.97	0.64
1:A:540:PHE:CD2	1:A:541:GLU:HG3	2.32	0.64
1:C:224:MET:HE3	1:C:224:MET:HA	1.79	0.64
1:D:533:ASP:OD2	1:D:612:LYS:HE2	1.98	0.64
1:F:255:LYS:O	1:F:256:GLU:HB2	1.97	0.64
1:B:584:GLN:HG3	1:B:598:THR:C	2.17	0.64
1:D:486:GLU:OE1	1:D:486:GLU:N	2.23	0.64
1:E:127:LEU:HD23	1:E:199:TYR:O	1.98	0.64
1:E:347:ASP:HB3	1:E:351:TYR:H	1.63	0.64
1:E:404:LEU:HD22	1:E:404:LEU:N	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:ILE:HD12	1:F:265:TRP:CD1	2.33	0.64
1:C:190:ASN:HD22	1:C:190:ASN:N	1.96	0.64
1:D:424:TRP:CE2	1:D:517:ILE:HD13	2.33	0.64
1:D:314:LEU:HD12	1:D:326:THR:HG22	1.80	0.63
1:B:632:LEU:HD13	1:B:634:GLN:HB2	1.78	0.63
1:D:127:LEU:CD1	1:D:196:GLU:HG2	2.27	0.63
1:F:586:LEU:N	1:F:586:LEU:HD23	2.13	0.63
1:A:341:ILE:HG22	1:B:632:LEU:HB2	1.78	0.63
1:E:118:GLN:HE22	1:E:322:ARG:H	1.45	0.63
1:F:301:ASP:OD2	1:F:303:HIS:NE2	2.31	0.63
1:F:332:VAL:HG13	1:F:442:TYR:CD2	2.32	0.63
1:D:211:VAL:HG22	1:D:242:ILE:HG12	1.78	0.63
1:E:373:ARG:HD2	1:E:373:ARG:O	1.98	0.63
1:F:239:LEU:HD13	1:F:268:LEU:HD11	1.81	0.63
1:A:200:TRP:HZ2	1:A:377:THR:HG21	1.64	0.63
1:A:449:GLY:CA	6:A:802:HOH:O	2.47	0.63
1:A:258:LEU:HD12	1:A:258:LEU:O	1.99	0.63
1:A:533:ASP:OD2	1:A:612:LYS:HE2	1.98	0.63
1:A:314:LEU:CD1	1:A:326:THR:CG2	2.76	0.63
1:F:454:ILE:O	1:F:457:GLY:N	2.32	0.63
1:B:628:ARG:HG2	1:B:649:TRP:CH2	2.34	0.62
1:C:207:LEU:CD1	1:C:319:SER:HA	2.29	0.62
1:A:632:LEU:CD2	1:B:342:PRO:HG2	2.27	0.62
1:C:180:SER:HB2	1:C:338:TYR:CZ	2.33	0.62
1:B:458:SER:HB3	1:B:463:LYS:HG3	1.81	0.62
1:C:151:GLU:HA	1:C:152:LYS:C	2.16	0.62
1:D:368:THR:HB	1:D:370:GLN:OE1	1.99	0.62
1:D:628:ARG:HG2	1:D:649:TRP:CH2	2.34	0.62
1:E:118:GLN:NE2	1:E:321:ASP:HA	2.14	0.62
1:C:485:PRO:HG3	1:C:531:ASN:ND2	2.14	0.62
1:F:200:TRP:HZ2	1:F:377:THR:HG21	1.65	0.62
1:B:456:VAL:HG23	1:B:457:GLY:C	2.20	0.62
1:B:414:GLY:HA2	1:B:415:GLU:OE2	2.00	0.62
1:F:299:TYR:O	1:F:391:LEU:HA	2.00	0.62
1:D:176:ASN:HD21	1:D:178:VAL:HG22	1.64	0.62
1:D:532:VAL:HB	1:D:573:ILE:HG23	1.82	0.62
1:D:122:TYR:CE1	1:D:203:ASP:HB3	2.35	0.62
1:B:255:LYS:O	1:B:256:GLU:HB2	2.00	0.61
1:B:212:VAL:HG22	1:B:299:TYR:CD1	2.36	0.61
1:B:584:GLN:CG	1:B:598:THR:O	2.42	0.61
1:C:332:VAL:HG13	1:C:442:TYR:HD2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:TYR:CZ	1:B:203:ASP:HB2	2.35	0.61
1:B:454:ILE:CG2	1:B:457:GLY:CA	2.50	0.61
1:C:565:MET:CE	1:D:163:LYS:HZ1	2.13	0.61
1:D:173:PHE:CD2	1:D:177:MET:HG3	2.34	0.61
1:F:368:THR:HB	1:F:370:GLN:OE1	1.99	0.61
1:C:255:LYS:O	1:C:256:GLU:HB2	1.98	0.61
1:C:485:PRO:O	1:C:488:GLN:HG3	1.99	0.61
1:D:377:THR:HG22	1:D:379:THR:H	1.65	0.61
1:C:414:GLY:HA2	1:C:415:GLU:OE2	2.00	0.61
1:C:546:ILE:CD1	1:C:626:LEU:HD21	2.30	0.61
1:E:514:MET:HE2	1:E:514:MET:HA	1.81	0.61
1:A:180:SER:OG	1:A:225:ARG:NH1	2.33	0.61
1:B:628:ARG:HH11	1:B:628:ARG:HG3	1.66	0.61
1:B:632:LEU:O	1:B:632:LEU:HD13	2.01	0.61
1:D:253:HIS:CD2	1:D:253:HIS:H	2.18	0.61
1:F:169:SER:HB2	1:F:177:MET:HB2	1.83	0.61
1:D:158:LEU:HD11	1:D:178:VAL:HG23	1.82	0.61
1:F:520:ASP:N	1:F:520:ASP:OD1	2.33	0.61
1:B:176:ASN:ND2	1:B:179:ALA:H	1.99	0.60
1:D:152:LYS:HD3	1:D:152:LYS:H	1.65	0.60
1:C:628:ARG:CG	1:C:628:ARG:HH11	2.14	0.60
1:E:176:ASN:HD22	1:E:176:ASN:C	2.04	0.60
1:E:533:ASP:OD2	1:E:612:LYS:HE2	2.02	0.60
1:F:377:THR:HG22	1:F:378:LYS:N	2.16	0.60
1:C:180:SER:OG	1:C:225:ARG:NH1	2.35	0.60
1:D:499:LYS:HE2	6:D:847:HOH:O	2.01	0.60
1:B:574:ASN:HB2	1:B:578:GLN:H	1.65	0.60
1:E:235:PRO:HB2	1:E:238:TYR:HD2	1.65	0.60
1:E:404:LEU:CD2	1:E:404:LEU:H	1.94	0.60
1:F:132:LEU:HD23	1:F:199:TYR:HE1	1.66	0.60
1:F:454:ILE:O	1:F:456:VAL:HA	2.01	0.60
1:B:314:LEU:HD12	1:B:326:THR:CG2	2.32	0.60
1:C:346:GLY:CA	1:C:366:PRO:HB3	2.28	0.60
1:D:490:LEU:HD12	1:D:490:LEU:C	2.20	0.60
1:D:641:ASP:H	1:D:647:GLN:NE2	1.99	0.60
1:C:159:GLY:HA2	1:C:162:PHE:H	1.66	0.60
1:D:191:ASP:OD1	1:D:193:ARG:HG2	2.01	0.60
1:E:459:SER:OG	1:E:460:PRO:HD3	1.99	0.60
1:F:453:PRO:CG	1:F:455:TYR:CZ	2.83	0.60
1:A:118:GLN:NE2	1:A:322:ARG:H	2.00	0.60
1:A:551:LYS:HE3	1:A:556:PHE:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ARG:NH1	1:B:308:VAL:HG22	2.17	0.60
1:C:546:ILE:HD11	1:C:626:LEU:HD21	1.83	0.60
1:D:251:LYS:HB2	1:D:254:LEU:HD22	1.83	0.60
1:C:628:ARG:NH1	1:C:646:THR:O	2.35	0.60
1:D:458:SER:HB3	1:D:463:LYS:NZ	2.17	0.60
1:B:514:MET:CE	1:B:514:MET:HA	2.28	0.59
1:E:551:LYS:HG2	1:E:555:GLY:HA3	1.84	0.59
1:B:128:ARG:HG3	1:B:201:HIS:CD2	2.37	0.59
1:E:118:GLN:HE22	1:E:322:ARG:N	1.99	0.59
1:A:159:GLY:HA2	1:A:162:PHE:H	1.66	0.59
1:A:574:ASN:HB2	1:A:578:GLN:H	1.66	0.59
1:E:208:THR:OG1	1:E:295:GLN:HG3	2.03	0.59
1:E:410:GLN:H	1:E:464:ASN:ND2	1.98	0.59
1:C:462:LEU:CD1	1:C:487:SER:HB3	2.28	0.59
1:A:619:HIS:CE1	1:A:621:PRO:HG2	2.38	0.59
1:B:131:ILE:O	1:B:199:TYR:HD1	1.85	0.59
1:D:280:LEU:HD13	4:D:702:UDP:H5'1	1.84	0.59
1:F:533:ASP:OD2	1:F:612:LYS:HE2	2.01	0.59
1:F:603:ASN:HA	1:F:606:LYS:HD2	1.85	0.59
1:A:406:ASP:HB2	1:A:498:LEU:HD21	1.85	0.59
1:A:627:ASP:OD1	1:A:646:THR:HB	2.03	0.59
1:B:314:LEU:CD1	1:B:326:THR:CG2	2.80	0.59
1:C:377:THR:HB	1:C:380:GLU:HG2	1.84	0.59
1:D:347:ASP:O	1:D:350:GLY:N	2.30	0.59
1:B:211:VAL:HA	1:B:298:ILE:O	2.03	0.59
1:C:246:ASP:OD1	1:C:249:SER:OG	2.20	0.58
1:C:628:ARG:HD2	1:C:646:THR:HG22	1.84	0.58
1:D:160:PRO:CA	1:D:163:LYS:HE3	2.32	0.58
1:F:254:LEU:O	1:F:273:ARG:NH2	2.36	0.58
1:A:154:LYS:HD2	6:A:874:HOH:O	2.04	0.58
1:A:347:ASP:HB3	1:A:351:TYR:N	2.16	0.58
1:A:513:PHE:CE1	1:A:517:ILE:HD11	2.38	0.58
1:C:551:LYS:HE3	1:C:556:PHE:O	2.04	0.58
1:F:212:VAL:HG21	1:F:299:TYR:CE2	2.38	0.58
1:C:332:VAL:HG22	1:C:442:TYR:CE2	2.38	0.58
1:F:180:SER:OG	1:F:225:ARG:NH1	2.36	0.58
1:B:314:LEU:O	1:B:326:THR:HG21	2.03	0.58
1:C:186:ASP:OD1	1:C:228:HIS:ND1	2.30	0.58
1:C:628:ARG:HG2	1:C:649:TRP:CH2	2.38	0.58
1:A:190:ASN:HD22	1:A:190:ASN:C	2.06	0.58
1:B:632:LEU:CD1	1:B:632:LEU:C	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ASN:HD22	1:D:190:ASN:C	2.05	0.58
1:C:276:ARG:HD2	1:C:278:GLU:OE2	2.04	0.58
1:D:485:PRO:HG3	1:D:531:ASN:ND2	2.18	0.58
1:F:207:LEU:CD1	1:F:319:SER:OG	2.52	0.58
1:A:580:MET:HG2	1:A:585:CYS:SG	2.44	0.58
1:C:390:GLY:C	1:C:391:LEU:HD23	2.24	0.58
1:C:455:TYR:HA	1:C:457:GLY:HA3	1.84	0.58
1:D:176:ASN:HD22	1:D:176:ASN:C	2.06	0.58
1:E:400:PHE:HA	1:E:404:LEU:HD13	1.85	0.58
1:B:485:PRO:HG3	1:B:531:ASN:ND2	2.19	0.58
1:C:414:GLY:HA3	1:C:416:ASN:H	1.69	0.58
1:D:127:LEU:HD11	1:D:196:GLU:CG	2.33	0.58
1:D:135:PHE:HE2	1:D:202:TYR:HB2	1.68	0.58
1:D:204:GLU:O	1:D:205:ASN:HB2	2.03	0.58
1:C:212:VAL:HG22	1:C:299:TYR:CD1	2.38	0.58
1:C:203:ASP:O	1:C:204:GLU:HB2	2.03	0.57
1:E:540:PHE:CD2	1:E:541:GLU:HG3	2.39	0.57
1:A:176:ASN:C	1:A:176:ASN:HD22	2.07	0.57
1:D:178:VAL:O	1:D:182:MET:HG2	2.04	0.57
1:A:449:GLY:N	6:A:802:HOH:O	2.32	0.57
1:D:251:LYS:HB2	1:D:254:LEU:CD2	2.33	0.57
1:E:255:LYS:O	1:E:256:GLU:HB2	2.04	0.57
1:F:627:ASP:HB3	1:F:636:PHE:CE1	2.38	0.57
1:D:377:THR:HG22	1:D:378:LYS:N	2.19	0.57
1:E:632:LEU:C	1:E:632:LEU:CD1	2.73	0.57
1:F:193:ARG:HE	1:F:197:CYS:CB	2.18	0.57
1:C:411:ILE:C	1:C:411:ILE:HD12	2.25	0.57
1:D:281:ILE:HD12	1:D:410:GLN:O	2.04	0.57
1:A:455:TYR:HB2	1:A:456:VAL:HG23	1.82	0.57
1:A:532:VAL:HB	1:A:573:ILE:HG23	1.86	0.57
1:C:454:ILE:O	1:C:457:GLY:CA	2.49	0.57
1:D:609:GLN:HG2	1:D:618:THR:CG2	2.33	0.57
1:F:454:ILE:C	1:F:457:GLY:H	2.07	0.57
1:B:176:ASN:C	1:B:176:ASN:HD22	2.08	0.57
1:C:314:LEU:O	1:C:326:THR:HG21	2.04	0.57
1:B:377:THR:HG22	1:B:378:LYS:N	2.20	0.57
1:B:641:ASP:OD1	1:B:643:SER:OG	2.23	0.57
1:D:373:ARG:NE	6:D:805:HOH:O	2.38	0.56
1:A:535:GLY:HA3	1:A:652:ASN:O	2.06	0.56
1:C:412:TRP:HE3	1:C:461:THR:HG21	1.70	0.56
1:F:264:LEU:HD23	1:F:264:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASP:O	1:A:204:GLU:HB2	2.05	0.56
1:A:467:ARG:NH2	1:A:495:ILE:HD12	2.20	0.56
1:B:212:VAL:CG2	1:B:299:TYR:CD1	2.88	0.56
1:E:314:LEU:CD1	1:E:326:THR:CG2	2.83	0.56
1:F:208:THR:OG1	1:F:295:GLN:HG3	2.04	0.56
1:A:332:VAL:HG13	1:A:442:TYR:CD2	2.38	0.56
1:F:196:GLU:CB	6:F:837:HOH:O	2.53	0.56
1:E:191:ASP:OD1	1:E:193:ARG:CG	2.53	0.56
1:F:632:LEU:HD11	1:F:634:GLN:HB2	1.86	0.56
1:B:118:GLN:HE22	1:B:322:ARG:N	2.00	0.56
1:B:422:LYS:HG2	1:B:472:TRP:HZ2	1.70	0.56
1:F:231:ILE:HD12	1:F:265:TRP:NE1	2.21	0.56
1:F:641:ASP:OD1	1:F:643:SER:OG	2.23	0.56
1:C:533:ASP:OD2	1:C:612:LYS:HE2	2.06	0.56
1:D:118:GLN:HE22	1:D:322:ARG:N	2.04	0.56
1:A:122:TYR:O	1:A:320:LYS:HG2	2.06	0.56
1:B:254:LEU:O	1:B:273:ARG:NH2	2.39	0.56
1:B:281:ILE:HD12	1:B:410:GLN:O	2.05	0.56
1:E:615:HIS:O	1:E:648:LYS:HA	2.05	0.56
1:A:325:CYS:HB2	1:A:394:ILE:HG23	1.88	0.56
1:F:152:LYS:O	1:F:188:SER:O	2.24	0.56
1:B:276:ARG:HD2	1:B:278:GLU:OE2	2.05	0.56
1:B:455:TYR:N	1:B:457:GLY:HA2	2.21	0.56
1:C:414:GLY:CA	1:C:415:GLU:HB3	2.21	0.56
1:A:235:PRO:HB2	1:A:238:TYR:HD2	1.70	0.56
1:B:347:ASP:HB3	1:B:351:TYR:N	2.17	0.56
1:C:574:ASN:HB2	1:C:578:GLN:H	1.71	0.56
1:F:574:ASN:HB2	1:F:578:GLN:H	1.69	0.56
1:C:207:LEU:HD13	1:C:319:SER:OG	2.06	0.55
1:D:127:LEU:HB2	1:D:200:TRP:CD2	2.41	0.55
1:D:332:VAL:HG13	1:D:442:TYR:HD2	1.70	0.55
1:C:479:TYR:CD1	1:C:528:PRO:HD2	2.41	0.55
1:C:629:SER:O	1:C:632:LEU:O	2.24	0.55
1:D:611:PHE:CD1	1:E:204:GLU:HB2	2.40	0.55
1:D:264:LEU:O	1:D:264:LEU:HD23	2.05	0.55
1:F:641:ASP:H	1:F:647:GLN:NE2	1.82	0.55
1:B:406:ASP:HB2	1:B:498:LEU:HD21	1.88	0.55
1:D:160:PRO:HA	1:D:163:LYS:CE	2.33	0.55
1:E:191:ASP:OD1	1:E:193:ARG:HG3	2.07	0.55
1:F:173:PHE:CD2	1:F:177:MET:HG3	2.41	0.55
1:A:306:VAL:HG21	1:A:310:TRP:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:O	1:A:326:THR:HG21	2.07	0.55
1:C:136:GLU:CD	1:C:193:ARG:HH22	2.06	0.55
1:C:406:ASP:HB2	1:C:498:LEU:HD21	1.88	0.55
1:E:189:VAL:HG12	1:E:190:ASN:O	2.06	0.55
1:E:118:GLN:NE2	1:E:322:ARG:H	2.03	0.55
1:F:414:GLY:CA	1:F:416:ASN:H	2.20	0.55
1:A:367:LEU:HD13	1:A:382:TYR:CD1	2.42	0.55
1:C:258:LEU:HD12	1:C:262:ILE:HG12	1.88	0.55
1:D:115:PHE:HE2	1:D:426:CYS:O	1.90	0.55
1:D:148:GLY:HA2	1:D:151:GLU:HG3	1.89	0.55
1:D:152:LYS:O	1:D:188:SER:O	2.23	0.55
1:F:178:VAL:O	1:F:182:MET:HG2	2.06	0.55
1:A:574:ASN:HB3	1:A:576:ALA:N	2.22	0.55
1:B:152:LYS:H	1:B:152:LYS:CD	2.18	0.55
1:A:368:THR:HB	1:A:370:GLN:OE1	2.07	0.55
1:D:627:ASP:HB3	1:D:636:PHE:CE1	2.42	0.55
1:F:193:ARG:NE	1:F:197:CYS:CB	2.67	0.55
1:C:584:GLN:HG2	1:C:599:HIS:HA	1.88	0.55
1:D:467:ARG:O	1:D:471:VAL:CG1	2.54	0.55
1:A:183:ILE:CG2	1:A:187:ARG:HD3	2.37	0.55
1:B:586:LEU:HA	1:B:596:MET:O	2.07	0.55
1:E:348:GLU:OE1	1:E:348:GLU:HA	2.07	0.55
1:F:200:TRP:CZ2	1:F:377:THR:HG21	2.42	0.55
1:B:485:PRO:O	1:B:488:GLN:CG	2.55	0.54
1:E:459:SER:CB	1:E:460:PRO:CD	2.85	0.54
1:F:627:ASP:OD1	1:F:646:THR:HB	2.06	0.54
1:A:301:ASP:OD2	1:A:440:HIS:NE2	2.38	0.54
1:E:603:ASN:HA	1:E:606:LYS:HD2	1.89	0.54
1:B:455:TYR:C	1:B:457:GLY:O	2.46	0.54
1:C:411:ILE:HD12	1:C:412:TRP:H	1.69	0.54
1:D:540:PHE:CD2	1:D:541:GLU:HG3	2.42	0.54
1:E:136:GLU:OE1	1:E:193:ARG:NH2	2.23	0.54
1:E:586:LEU:H	1:E:586:LEU:HD23	1.73	0.54
1:B:603:ASN:HA	1:B:606:LYS:HD2	1.89	0.54
1:C:113:LEU:HD12	1:C:504:ASP:HB3	1.88	0.54
1:C:455:TYR:HD1	1:C:455:TYR:H	1.54	0.54
1:E:485:PRO:HG3	1:E:531:ASN:ND2	2.22	0.54
1:F:641:ASP:N	1:F:647:GLN:HE22	1.83	0.54
1:A:151:GLU:HA	1:A:153:ALA:H	1.72	0.54
1:A:167:GLN:NE2	6:A:805:HOH:O	2.41	0.54
1:D:116:LYS:NZ	1:D:397:GLU:HG2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:SER:OG	1:E:225:ARG:NH1	2.41	0.54
1:F:551:LYS:HE3	1:F:556:PHE:O	2.08	0.54
1:C:176:ASN:ND2	1:C:179:ALA:H	2.06	0.54
1:E:175:PHE:CE1	1:E:441:ILE:HG22	2.43	0.54
1:A:241:GLU:OE1	1:A:293:LEU:HD22	2.08	0.54
1:A:118:GLN:HE22	1:A:322:ARG:N	2.06	0.54
1:B:231:ILE:HD12	1:B:265:TRP:CD1	2.43	0.54
1:B:456:VAL:CA	1:B:457:GLY:C	2.76	0.54
1:F:132:LEU:HD23	1:F:199:TYR:CE1	2.43	0.54
1:B:231:ILE:HD12	1:B:265:TRP:NE1	2.23	0.54
1:B:456:VAL:HG22	1:B:458:SER:HA	1.78	0.54
1:B:610:TYR:HB2	1:B:617:PHE:CE1	2.42	0.54
1:C:632:LEU:HD11	1:C:634:GLN:CD	2.28	0.54
1:A:586:LEU:HD23	1:A:586:LEU:N	2.23	0.53
1:C:299:TYR:O	1:C:300:LEU:HD13	2.08	0.53
1:C:312:ALA:HB3	1:C:313:PRO:HD3	1.89	0.53
1:C:348:GLU:OE1	1:C:348:GLU:HA	2.08	0.53
1:C:332:VAL:HG13	1:C:442:TYR:CD2	2.43	0.53
1:D:158:LEU:HD12	1:D:178:VAL:CG2	2.38	0.53
1:D:628:ARG:HH11	1:D:628:ARG:CG	2.20	0.53
1:D:410:GLN:HB2	1:D:460:PRO:HB2	1.89	0.53
1:F:151:GLU:HA	1:F:152:LYS:O	2.08	0.53
1:F:322:ARG:NH1	1:F:401:GLU:OE1	2.40	0.53
1:A:449:GLY:HA2	6:A:802:HOH:O	2.07	0.53
1:A:604:GLU:HG2	6:A:847:HOH:O	2.07	0.53
1:B:447:TRP:O	1:B:448:GLN:HG2	2.09	0.53
1:B:312:ALA:HB3	1:B:313:PRO:HD3	1.91	0.53
1:C:200:TRP:HZ2	1:C:377:THR:HG21	1.74	0.53
1:F:190:ASN:HD22	1:F:190:ASN:C	2.11	0.53
1:A:286:ILE:HG22	1:A:290:LYS:HD2	1.89	0.53
1:B:141:GLU:OE1	1:B:232:LYS:NZ	2.31	0.53
1:B:279:GLY:HA2	1:B:411:ILE:HD12	1.90	0.53
1:B:454:ILE:HG21	1:B:457:GLY:HA3	1.81	0.53
1:C:176:ASN:C	1:C:176:ASN:HD22	2.10	0.53
1:E:152:LYS:CD	1:E:152:LYS:H	2.21	0.53
1:E:628:ARG:HG2	1:E:649:TRP:CH2	2.44	0.53
1:D:116:LYS:O	1:D:322:ARG:NH2	2.42	0.53
1:A:176:ASN:ND2	1:A:179:ALA:H	2.06	0.53
1:A:212:VAL:HG21	1:A:299:TYR:CE1	2.43	0.53
1:A:458:SER:N	1:A:459:SER:CA	2.72	0.53
1:B:180:SER:OG	1:B:225:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:CYS:HB2	1:C:394:ILE:CG2	2.38	0.53
1:E:559:LEU:O	1:E:633:HIS:HB3	2.07	0.53
1:C:314:LEU:HD11	1:C:326:THR:HG22	1.90	0.53
1:C:414:GLY:CA	1:C:416:ASN:H	2.21	0.53
1:C:522:THR:HG22	1:C:527:LEU:HD13	1.91	0.53
1:A:266:ASN:HD21	1:D:500:LYS:NZ	2.07	0.53
1:F:551:LYS:HG2	1:F:555:GLY:HA3	1.91	0.53
1:A:118:GLN:HE22	1:A:322:ARG:H	1.56	0.52
1:B:533:ASP:OD2	1:B:612:LYS:HE2	2.09	0.52
1:C:207:LEU:HD11	1:C:319:SER:HA	1.90	0.52
1:C:565:MET:CE	1:D:163:LYS:NZ	2.73	0.52
1:D:207:LEU:CD1	1:D:319:SER:OG	2.56	0.52
1:E:190:ASN:HD22	1:E:190:ASN:C	2.12	0.52
1:E:254:LEU:O	1:E:273:ARG:NH2	2.42	0.52
1:E:455:TYR:CB	1:E:456:VAL:HG22	2.35	0.52
1:A:332:VAL:HG22	1:A:442:TYR:CE2	2.44	0.52
1:D:314:LEU:CD1	1:D:326:THR:CG2	2.86	0.52
1:D:118:GLN:HE22	1:D:322:ARG:H	1.54	0.52
1:D:535:GLY:HA3	1:D:652:ASN:O	2.09	0.52
1:F:559:LEU:O	1:F:633:HIS:HB3	2.10	0.52
1:F:163:LYS:HG3	1:F:164:GLN:N	2.23	0.52
1:A:200:TRP:CZ2	1:A:377:THR:HG21	2.44	0.52
1:A:457:GLY:HA3	1:A:459:SER:OG	2.09	0.52
1:A:356:TRP:HZ2	1:A:514:MET:HE3	1.75	0.52
1:D:127:LEU:HB2	1:D:200:TRP:CE3	2.44	0.52
1:D:536:GLU:HA	1:D:569:GLN:O	2.10	0.52
1:E:551:LYS:HE3	1:E:556:PHE:O	2.09	0.52
1:E:628:ARG:HH11	1:E:628:ARG:CG	2.22	0.52
1:E:641:ASP:HB3	1:E:644:LYS:HG3	1.92	0.52
1:F:454:ILE:HG23	1:F:457:GLY:HA3	1.90	0.52
1:F:547:ASP:HB2	1:F:569:GLN:CG	2.26	0.52
1:A:152:LYS:HD2	1:A:152:LYS:N	2.25	0.52
1:D:574:ASN:HB3	1:D:576:ALA:H	1.75	0.52
1:E:411:ILE:N	1:E:411:ILE:CD1	2.73	0.52
1:F:356:TRP:HZ2	1:F:514:MET:HE3	1.75	0.52
1:A:576:ALA:O	1:A:577:ASN:HB2	2.10	0.52
1:B:576:ALA:O	1:B:577:ASN:HB2	2.10	0.52
1:B:628:ARG:HH11	1:B:628:ARG:CG	2.22	0.52
1:C:132:LEU:HD23	1:C:199:TYR:CE1	2.44	0.52
1:C:301:ASP:OD2	1:C:440:HIS:NE2	2.32	0.52
1:C:282:GLN:CG	1:C:410:GLN:NE2	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:632:LEU:HD22	1:E:633:HIS:N	2.24	0.52
1:A:424:TRP:CE2	1:A:517:ILE:HD13	2.45	0.52
1:D:603:ASN:O	1:D:606:LYS:HD2	2.09	0.52
1:E:152:LYS:CD	1:E:152:LYS:N	2.73	0.52
1:E:641:ASP:H	1:E:647:GLN:NE2	1.95	0.52
1:F:326:THR:HG23	1:F:433:VAL:CG2	2.40	0.52
1:F:540:PHE:O	1:F:542:THR:HG23	2.09	0.52
1:B:311:TYR:CZ	1:B:315:VAL:HG21	2.45	0.51
1:B:455:TYR:N	1:B:455:TYR:CD1	2.73	0.51
1:B:620:ILE:N	1:B:621:PRO:HD2	2.25	0.51
1:C:218:GLU:O	1:C:253:HIS:HE1	1.93	0.51
1:D:136:GLU:OE2	1:D:193:ARG:NH2	2.43	0.51
1:F:632:LEU:C	1:F:632:LEU:CD1	2.78	0.51
1:F:641:ASP:HB3	1:F:644:LYS:HG3	1.90	0.51
1:B:314:LEU:HD11	1:B:328:PRO:HD3	1.92	0.51
1:B:611:PHE:HB3	1:B:614:LEU:HB2	1.91	0.51
1:E:371:GLU:HG2	1:E:519:TYR:OH	2.09	0.51
1:F:453:PRO:CG	1:F:455:TYR:OH	2.58	0.51
1:A:239:LEU:HD13	1:A:268:LEU:HD11	1.92	0.51
1:D:473:TRP:CZ3	1:D:480:PHE:HB2	2.44	0.51
1:A:152:LYS:CD	1:A:152:LYS:N	2.73	0.51
1:C:514:MET:HE2	1:C:514:MET:HA	1.92	0.51
1:D:251:LYS:HB2	1:D:253:HIS:NE2	2.25	0.51
1:E:574:ASN:HB3	1:E:576:ALA:H	1.76	0.51
1:A:152:LYS:CD	1:A:152:LYS:H	2.24	0.51
1:F:314:LEU:O	1:F:326:THR:HG21	2.10	0.51
1:A:410:GLN:N	1:A:464:ASN:HD21	2.09	0.51
1:B:632:LEU:HD11	1:B:634:GLN:CG	2.41	0.51
1:D:629:SER:HG	1:D:632:LEU:HD13	1.75	0.51
1:F:453:PRO:HB3	1:F:455:TYR:CZ	2.40	0.51
1:A:306:VAL:HG21	1:A:310:TRP:CE2	2.46	0.51
1:B:212:VAL:CG2	1:B:299:TYR:CE1	2.93	0.51
1:C:190:ASN:H	1:C:190:ASN:HD22	1.58	0.51
1:C:641:ASP:H	1:C:647:GLN:NE2	1.90	0.51
1:D:367:LEU:HD13	1:D:382:TYR:CD1	2.46	0.51
1:E:584:GLN:HG2	1:E:599:HIS:HA	1.92	0.51
1:A:264:LEU:O	1:A:264:LEU:HD22	2.11	0.51
1:A:548:SER:CB	1:A:581:GLN:OE1	2.59	0.51
1:B:264:LEU:O	1:B:264:LEU:HD22	2.11	0.51
1:C:347:ASP:HB3	1:C:351:TYR:N	2.25	0.51
1:E:116:LYS:O	1:E:322:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:THR:HB	1:E:370:GLN:OE1	2.11	0.51
1:B:513:PHE:CE1	1:B:517:ILE:HD11	2.46	0.50
1:C:632:LEU:C	1:C:632:LEU:CD1	2.76	0.50
1:D:586:LEU:HD23	1:D:597:ILE:HG12	1.92	0.50
1:F:390:GLY:C	1:F:391:LEU:HD23	2.31	0.50
1:B:190:ASN:C	1:B:190:ASN:HD22	2.11	0.50
1:D:586:LEU:CD2	1:D:597:ILE:HG13	2.41	0.50
1:E:231:ILE:HD12	1:E:265:TRP:NE1	2.26	0.50
1:A:641:ASP:OD1	1:A:643:SER:OG	2.28	0.50
1:B:563:HIS:O	1:B:565:MET:HG2	2.10	0.50
1:C:462:LEU:HD12	1:C:490:LEU:HD22	1.92	0.50
1:D:118:GLN:NE2	1:D:322:ARG:N	2.58	0.50
1:D:254:LEU:O	1:D:258:LEU:HB2	2.11	0.50
1:E:346:GLY:HA3	1:E:366:PRO:CA	2.40	0.50
1:E:387:MET:HG3	1:E:387:MET:O	2.11	0.50
1:F:193:ARG:HG2	1:F:197:CYS:SG	2.49	0.50
1:A:314:LEU:HD12	1:A:326:THR:HG22	1.82	0.50
1:A:549:MET:HB2	1:A:551:LYS:HD3	1.94	0.50
1:E:619:HIS:NE2	1:E:621:PRO:HG2	2.26	0.50
1:E:629:SER:O	1:E:632:LEU:O	2.30	0.50
1:B:500:LYS:NZ	1:C:266:ASN:HD21	2.10	0.50
1:D:406:ASP:OD1	1:D:408:GLY:N	2.43	0.50
1:B:540:PHE:CD2	1:B:541:GLU:HG3	2.47	0.50
1:B:629:SER:O	1:B:632:LEU:O	2.29	0.50
1:B:627:ASP:HB3	1:B:636:PHE:CE1	2.46	0.50
1:C:211:VAL:HG22	1:C:242:ILE:HG23	1.94	0.50
1:F:211:VAL:HA	1:F:298:ILE:O	2.12	0.50
1:B:551:LYS:HE3	1:B:556:PHE:O	2.12	0.50
1:C:485:PRO:HG3	1:C:531:ASN:HD21	1.75	0.50
1:D:321:ASP:HB3	1:D:324:ILE:HD12	1.93	0.50
1:F:411:ILE:CD1	1:F:460:PRO:HG2	2.42	0.50
1:A:128:ARG:HG3	1:A:201:HIS:CD2	2.47	0.50
1:A:377:THR:HG22	1:A:379:THR:N	2.12	0.50
1:A:581:GLN:HG2	1:A:582:TYR:CD2	2.47	0.50
1:C:152:LYS:O	1:C:188:SER:O	2.30	0.50
1:E:122:TYR:O	1:E:320:LYS:HG2	2.12	0.50
1:E:172:GLU:HG3	1:E:251:LYS:NZ	2.26	0.50
1:F:193:ARG:HG2	1:F:197:CYS:HB2	1.93	0.50
1:F:629:SER:O	1:F:632:LEU:O	2.30	0.50
1:B:172:GLU:CG	1:B:251:LYS:HZ3	2.24	0.50
1:B:520:ASP:OD1	1:B:520:ASP:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HD13	1:C:319:SER:HA	1.93	0.49
1:E:332:VAL:HG13	1:E:442:TYR:HD2	1.77	0.49
1:B:127:LEU:HD23	1:B:199:TYR:O	2.12	0.49
1:B:377:THR:CG2	1:B:378:LYS:N	2.75	0.49
1:E:632:LEU:HD11	1:E:634:GLN:CD	2.32	0.49
1:B:116:LYS:NZ	1:B:397:GLU:OE1	2.45	0.49
1:B:218:GLU:O	1:B:253:HIS:HE1	1.96	0.49
1:B:424:TRP:CE2	1:B:517:ILE:HD13	2.47	0.49
1:F:453:PRO:HB2	1:F:455:TYR:CE1	2.33	0.49
1:D:207:LEU:HD12	1:D:207:LEU:N	2.28	0.49
1:A:127:LEU:HD23	1:A:199:TYR:O	2.13	0.49
1:A:258:LEU:HD12	1:A:258:LEU:C	2.32	0.49
1:D:206:LEU:HD12	1:D:238:TYR:CE2	2.47	0.49
1:A:231:ILE:HD12	1:A:265:TRP:CD1	2.47	0.49
1:A:348:GLU:HA	1:A:348:GLU:OE1	2.12	0.49
1:B:152:LYS:N	1:B:152:LYS:CD	2.76	0.49
1:B:615:HIS:O	1:B:648:LYS:HA	2.13	0.49
1:C:447:TRP:C	1:C:448:GLN:HG2	2.32	0.49
1:D:276:ARG:NH1	1:D:278:GLU:OE1	2.45	0.49
1:D:346:GLY:HA3	1:D:366:PRO:HB3	1.93	0.49
1:E:176:ASN:ND2	1:E:179:ALA:H	2.10	0.49
1:E:224:MET:CE	1:E:224:MET:HA	2.40	0.49
1:E:285:SER:O	1:E:289:GLN:HG3	2.13	0.49
1:A:215:PHE:CE1	1:A:254:LEU:HD22	2.46	0.49
1:B:122:TYR:CE1	1:B:203:ASP:HB3	2.47	0.49
1:C:457:GLY:HA2	1:C:458:SER:C	2.32	0.49
1:D:418:GLU:HG3	1:D:468:VAL:HG22	1.93	0.49
1:E:347:ASP:HB3	1:E:351:TYR:N	2.28	0.49
1:F:312:ALA:HB3	1:F:313:PRO:HD3	1.93	0.49
1:B:535:GLY:HA3	1:B:652:ASN:O	2.12	0.49
1:C:586:LEU:HD23	1:C:586:LEU:H	1.73	0.49
1:A:286:ILE:HG23	1:A:290:LYS:HD2	1.95	0.49
1:A:281:ILE:CD1	1:A:415:GLU:CG	2.91	0.49
1:B:447:TRP:C	1:B:448:GLN:HG2	2.33	0.49
1:B:450:ASN:N	1:B:450:ASN:ND2	2.59	0.49
1:D:153:ALA:HB2	1:D:190:ASN:HB3	1.94	0.49
1:E:414:GLY:CA	1:E:416:ASN:N	2.74	0.49
1:A:150:GLY:O	1:A:153:ALA:HA	2.13	0.48
1:A:304:CYS:HA	1:A:439:GLY:O	2.13	0.48
1:B:406:ASP:OD2	1:B:409:LEU:HD13	2.13	0.48
1:C:462:LEU:HD11	1:C:487:SER:CB	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:GLU:HA	1:C:569:GLN:O	2.13	0.48
1:D:134:ASN:N	1:D:134:ASN:OD1	2.40	0.48
1:F:301:ASP:OD2	1:F:440:HIS:NE2	2.36	0.48
1:B:200:TRP:HZ2	1:B:377:THR:HG21	1.78	0.48
1:C:211:VAL:HA	1:C:298:ILE:O	2.12	0.48
1:D:160:PRO:HA	1:D:163:LYS:CG	2.41	0.48
1:D:607:GLU:HB2	1:D:621:PRO:HD3	1.93	0.48
1:F:301:ASP:H	1:F:391:LEU:CD2	2.26	0.48
1:D:160:PRO:O	1:D:163:LYS:HG3	2.13	0.48
1:A:254:LEU:O	1:A:273:ARG:NH2	2.46	0.48
1:A:325:CYS:HB3	1:A:423:ILE:HD13	1.95	0.48
1:B:394:ILE:HG22	6:B:811:HOH:O	2.13	0.48
1:E:200:TRP:HZ2	1:E:377:THR:HG21	1.78	0.48
1:A:394:ILE:HD12	1:A:399:PHE:HB2	1.95	0.48
1:D:278:GLU:HG3	1:D:286:ILE:HD11	1.95	0.48
1:E:314:LEU:HD11	1:E:326:THR:HG22	1.96	0.48
1:F:176:ASN:HD22	1:F:176:ASN:C	2.17	0.48
1:F:180:SER:HB2	1:F:338:TYR:CZ	2.48	0.48
1:A:209:SER:OG	1:A:296:VAL:HG22	2.13	0.48
1:D:186:ASP:OD1	1:D:228:HIS:ND1	2.46	0.48
1:F:194:GLN:O	1:F:197:CYS:HB2	2.14	0.48
1:F:485:PRO:HG3	1:F:531:ASN:ND2	2.29	0.48
1:F:628:ARG:CG	1:F:628:ARG:HH11	2.25	0.48
1:C:212:VAL:HG21	1:C:299:TYR:CE1	2.49	0.48
1:C:375:ARG:NE	1:C:382:TYR:HB3	2.28	0.48
1:D:406:ASP:HB2	1:D:498:LEU:HD11	1.95	0.48
1:F:377:THR:CG2	1:F:378:LYS:N	2.77	0.48
1:A:225:ARG:O	1:A:229:SER:HB3	2.13	0.48
1:A:587:THR:OG1	1:A:588:LYS:N	2.45	0.48
1:B:454:ILE:HD12	1:B:460:PRO:HG2	1.96	0.48
1:D:458:SER:HB3	1:D:463:LYS:HZ1	1.78	0.48
1:E:235:PRO:HB2	1:E:238:TYR:CD2	2.46	0.48
1:F:603:ASN:CA	1:F:606:LYS:HD2	2.43	0.48
1:A:371:GLU:HG2	1:A:519:TYR:OH	2.14	0.48
1:B:620:ILE:H	1:B:621:PRO:HD2	1.79	0.48
1:C:385:PRO:HA	1:C:517:ILE:CD1	2.44	0.48
1:C:513:PHE:CD1	1:C:517:ILE:HG12	2.49	0.48
1:D:158:LEU:HD12	1:D:166:ILE:HD11	1.96	0.48
1:E:532:VAL:HB	1:E:573:ILE:HG23	1.94	0.48
1:E:583:ASP:OD2	1:E:599:HIS:HD2	1.95	0.48
1:A:281:ILE:CD1	1:A:415:GLU:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:TYR:CE1	1:B:203:ASP:CB	2.97	0.48
1:B:456:VAL:CG2	1:B:457:GLY:C	2.83	0.48
1:B:579:LEU:HB2	1:B:608:TRP:CD1	2.49	0.48
1:C:264:LEU:HD13	1:C:265:TRP:CE2	2.48	0.48
1:F:453:PRO:O	1:F:455:TYR:CD2	2.66	0.48
1:A:458:SER:HG	1:A:462:LEU:HB2	1.77	0.47
1:A:554:GLY:O	1:A:596:MET:HG3	2.14	0.47
1:F:412:TRP:O	1:F:461:THR:HB	2.13	0.47
1:A:314:LEU:HD11	1:A:326:THR:HG22	1.92	0.47
1:C:187:ARG:HG3	1:C:187:ARG:O	2.14	0.47
1:D:373:ARG:HD2	6:D:805:HOH:O	2.13	0.47
1:B:400:PHE:O	1:B:403:GLY:HA3	2.15	0.47
1:B:447:TRP:CD1	1:B:448:GLN:N	2.81	0.47
1:C:193:ARG:NH1	1:C:308:VAL:HG22	2.29	0.47
1:D:239:LEU:HD13	1:D:268:LEU:HD11	1.96	0.47
1:D:373:ARG:NH1	6:D:805:HOH:O	2.46	0.47
1:E:514:MET:HE1	1:E:518:ALA:CB	2.44	0.47
1:E:539:GLY:CA	1:E:628:ARG:NH2	2.77	0.47
1:A:485:PRO:HG3	1:A:531:ASN:ND2	2.29	0.47
1:B:191:ASP:OD1	1:B:193:ARG:CG	2.62	0.47
1:D:347:ASP:CB	1:D:351:TYR:H	2.03	0.47
1:E:603:ASN:CA	1:E:606:LYS:HD2	2.45	0.47
1:F:192:LEU:HD11	1:F:340:ILE:HG22	1.94	0.47
1:A:262:ILE:HA	1:A:262:ILE:HD13	1.56	0.47
1:A:447:TRP:C	1:A:448:GLN:HG2	2.35	0.47
1:A:459:SER:HB3	1:A:460:PRO:HD3	1.94	0.47
1:B:631:VAL:O	1:B:631:VAL:HG23	2.15	0.47
1:F:356:TRP:HZ2	1:F:514:MET:CE	2.27	0.47
1:F:116:LYS:NZ	1:F:397:GLU:OE1	2.46	0.47
1:A:510:PHE:CZ	1:A:514:MET:HE3	2.49	0.47
1:B:346:GLY:N	6:B:807:HOH:O	2.48	0.47
1:B:641:ASP:HB3	1:B:644:LYS:HG3	1.96	0.47
1:D:458:SER:O	1:D:459:SER:C	2.52	0.47
1:E:367:LEU:HD13	1:E:382:TYR:CD1	2.49	0.47
1:E:450:ASN:H	1:E:450:ASN:HD22	1.60	0.47
1:C:212:VAL:CG2	1:C:299:TYR:CE1	2.98	0.47
1:C:586:LEU:CD2	1:C:586:LEU:N	2.76	0.47
1:E:375:ARG:NE	1:E:382:TYR:HB3	2.29	0.47
1:A:306:VAL:CG2	1:A:310:TRP:CD2	2.98	0.47
1:A:602:LEU:HD23	1:A:602:LEU:HA	1.55	0.47
1:B:203:ASP:O	1:B:204:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLU:OE1	1:C:293:LEU:HD22	2.13	0.47
1:C:378:LYS:HB3	1:C:378:LYS:HE3	1.65	0.47
1:C:553:ASN:HA	1:C:598:THR:HA	1.96	0.47
1:E:620:ILE:H	1:E:621:PRO:HD2	1.80	0.47
1:A:394:ILE:HD12	1:A:399:PHE:CG	2.49	0.47
1:A:502:ARG:HG3	1:A:507:CYS:HB2	1.97	0.47
1:D:413:GLY:HA2	3:D:701:NAG:O6	2.15	0.47
1:E:414:GLY:CA	1:E:415:GLU:CB	2.83	0.47
1:F:207:LEU:HD11	1:F:319:SER:HA	1.96	0.47
1:F:235:PRO:HB2	1:F:238:TYR:HD2	1.80	0.47
1:F:400:PHE:HA	1:F:404:LEU:CD1	2.45	0.47
1:A:373:ARG:O	1:A:373:ARG:CD	2.63	0.47
1:C:346:GLY:N	6:C:801:HOH:O	2.47	0.47
1:E:380:GLU:HB2	1:E:381:PRO:CD	2.45	0.47
1:F:146:VAL:HA	1:F:147:GLY:HA2	1.64	0.47
1:F:193:ARG:HG2	1:F:197:CYS:CB	2.45	0.47
1:F:207:LEU:HD13	1:F:319:SER:OG	2.14	0.47
1:B:377:THR:HG22	1:B:379:THR:N	2.17	0.47
1:B:616:ARG:HG2	1:B:618:THR:HG22	1.97	0.47
1:C:322:ARG:HH11	1:C:397:GLU:HB3	1.78	0.47
1:E:620:ILE:N	1:E:621:PRO:HD2	2.30	0.47
1:F:180:SER:HB2	1:F:338:TYR:OH	2.15	0.47
1:F:346:GLY:HA3	1:F:366:PRO:HB3	1.95	0.47
1:F:586:LEU:HA	1:F:596:MET:O	2.15	0.47
1:B:314:LEU:HD12	1:B:326:THR:HG23	1.95	0.46
1:E:156:LEU:O	1:E:337:THR:HG22	2.14	0.46
1:F:122:TYR:OH	1:F:206:LEU:CD2	2.64	0.46
1:F:118:GLN:NE2	1:F:322:ARG:H	2.12	0.46
1:C:122:TYR:CZ	1:C:203:ASP:CB	2.95	0.46
1:C:602:LEU:HA	1:C:602:LEU:HD23	1.66	0.46
1:D:153:ALA:CB	1:D:190:ASN:HB3	2.45	0.46
1:F:212:VAL:CG2	1:F:299:TYR:CD2	2.97	0.46
1:F:453:PRO:HB3	1:F:455:TYR:OH	2.15	0.46
1:A:212:VAL:HG22	1:A:299:TYR:CD1	2.50	0.46
1:B:402:LEU:HD23	1:B:402:LEU:HA	1.75	0.46
1:B:586:LEU:CD2	1:B:586:LEU:N	2.76	0.46
1:C:208:THR:O	1:C:296:VAL:HG13	2.16	0.46
1:D:499:LYS:HG3	6:D:816:HOH:O	2.13	0.46
1:F:411:ILE:CG2	1:F:412:TRP:N	2.73	0.46
1:A:211:VAL:HG22	1:A:242:ILE:HG12	1.97	0.46
1:B:262:ILE:HA	1:B:262:ILE:HD13	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:ALA:O	1:C:577:ASN:HB2	2.16	0.46
1:C:593:SER:HB3	1:C:637:ILE:O	2.15	0.46
1:C:627:ASP:OD1	1:C:646:THR:HB	2.15	0.46
1:D:180:SER:OG	1:D:225:ARG:NH1	2.49	0.46
1:D:231:ILE:HD12	1:D:265:TRP:CD1	2.50	0.46
1:D:632:LEU:N	1:D:632:LEU:HD12	2.31	0.46
1:E:410:GLN:O	1:E:412:TRP:N	2.43	0.46
1:F:456:VAL:O	1:F:456:VAL:HG12	2.15	0.46
1:F:474:ASP:O	1:F:477:LYS:HG2	2.15	0.46
1:A:315:VAL:HG12	1:A:315:VAL:O	2.15	0.46
1:B:610:TYR:OH	1:B:612:LYS:HG3	2.16	0.46
1:C:490:LEU:HD12	1:C:656:SER:O	2.15	0.46
1:E:183:ILE:O	1:E:225:ARG:NH2	2.49	0.46
1:E:377:THR:HG22	1:E:378:LYS:N	2.31	0.46
1:F:138:LYS:HB2	1:F:138:LYS:HE3	1.62	0.46
1:F:316:ALA:N	1:F:317:PRO:HD2	2.30	0.46
1:A:258:LEU:CD1	1:A:262:ILE:HG12	2.45	0.46
1:A:474:ASP:O	1:A:477:LYS:HG2	2.15	0.46
1:A:513:PHE:CD2	1:A:514:MET:HE2	2.51	0.46
1:C:286:ILE:CG2	1:C:290:LYS:HD2	2.45	0.46
1:C:447:TRP:C	1:C:448:GLN:CG	2.84	0.46
1:D:225:ARG:O	1:D:229:SER:HB3	2.16	0.46
1:E:212:VAL:HG21	1:E:299:TYR:CE2	2.50	0.46
1:E:455:TYR:HA	1:E:456:VAL:HA	1.62	0.46
1:E:602:LEU:HD22	1:E:602:LEU:O	2.15	0.46
1:F:113:LEU:HD12	1:F:504:ASP:HB3	1.98	0.46
1:A:192:LEU:HD22	1:A:342:PRO:HD3	1.98	0.46
1:A:463:LYS:HE3	1:A:463:LYS:HB2	1.63	0.46
1:A:548:SER:HB2	1:A:581:GLN:OE1	2.16	0.46
1:B:235:PRO:HB2	1:B:238:TYR:HD2	1.80	0.46
1:B:316:ALA:HB3	1:B:317:PRO:HD3	1.98	0.46
1:B:385:PRO:HA	1:B:517:ILE:HD11	1.98	0.46
1:C:455:TYR:HA	1:C:456:VAL:HA	1.42	0.46
1:E:409:LEU:HD13	1:E:415:GLU:HB2	1.97	0.46
1:C:476:TYR:CE2	1:C:514:MET:HG3	2.50	0.46
1:D:586:LEU:HD23	1:D:597:ILE:CG1	2.46	0.46
1:E:200:TRP:CZ2	1:E:377:THR:HG21	2.51	0.46
1:E:632:LEU:O	1:E:632:LEU:HD13	2.16	0.46
1:B:314:LEU:HG	1:B:326:THR:HG21	1.98	0.46
1:E:574:ASN:ND2	1:E:578:GLN:OE1	2.49	0.46
1:E:614:LEU:HD23	1:E:614:LEU:HA	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:ARG:HB3	1:F:131:ILE:HD12	1.97	0.46
1:F:195:GLU:OE2	1:F:198:LYS:HE3	2.16	0.46
1:F:454:ILE:CG2	1:F:457:GLY:O	2.63	0.46
1:A:312:ALA:N	1:A:313:PRO:CD	2.78	0.46
1:B:549:MET:HB2	1:B:551:LYS:HD3	1.98	0.46
1:C:447:TRP:CD1	1:C:448:GLN:N	2.83	0.46
1:C:450:ASN:HD22	1:C:450:ASN:H	1.63	0.46
1:D:231:ILE:HD12	1:D:265:TRP:NE1	2.31	0.46
1:D:588:LYS:HD2	1:D:589:GLY:O	2.15	0.46
1:A:422:LYS:HG2	1:A:472:TRP:HZ2	1.76	0.45
1:A:574:ASN:ND2	1:A:578:GLN:OE1	2.49	0.45
1:A:627:ASP:HB3	1:A:636:PHE:CE1	2.51	0.45
1:B:138:LYS:HB2	1:B:138:LYS:HE3	1.61	0.45
1:C:373:ARG:O	1:C:373:ARG:HD2	2.16	0.45
1:E:485:PRO:O	1:E:488:GLN:HG3	2.16	0.45
1:F:615:HIS:O	1:F:648:LYS:HA	2.17	0.45
1:A:138:LYS:HE3	1:A:138:LYS:HB2	1.52	0.45
1:A:394:ILE:HD12	1:A:399:PHE:CB	2.46	0.45
1:B:172:GLU:HG2	1:B:251:LYS:HZ3	1.82	0.45
1:C:321:ASP:HB3	1:C:324:ILE:HG13	1.97	0.45
1:D:189:VAL:HG12	1:D:190:ASN:O	2.16	0.45
1:B:146:VAL:HA	1:B:147:GLY:HA2	1.56	0.45
1:B:118:GLN:NE2	1:B:321:ASP:HA	2.30	0.45
1:C:391:LEU:HD23	1:C:391:LEU:N	2.31	0.45
1:D:160:PRO:N	1:D:161:GLU:OE2	2.49	0.45
1:C:163:LYS:NZ	5:D:704:UD2:O2A	2.49	0.45
1:E:138:LYS:HB2	1:E:138:LYS:HE3	1.71	0.45
1:E:194:GLN:O	1:E:197:CYS:HB2	2.16	0.45
1:F:455:TYR:HA	1:F:456:VAL:HA	1.65	0.45
1:B:474:ASP:O	1:B:477:LYS:HG2	2.17	0.45
1:C:116:LYS:NZ	1:C:397:GLU:HG2	2.32	0.45
1:C:574:ASN:HB3	1:C:576:ALA:N	2.29	0.45
1:E:172:GLU:HG3	1:E:251:LYS:HZ1	1.81	0.45
1:F:122:TYR:CD2	1:F:205:ASN:HB3	2.52	0.45
1:A:380:GLU:HB2	1:A:381:PRO:HD2	1.97	0.45
1:B:517:ILE:HG13	1:B:518:ALA:N	2.32	0.45
1:D:418:GLU:OE2	6:D:801:HOH:O	2.21	0.45
1:F:179:ALA:O	1:F:183:ILE:HG13	2.16	0.45
1:F:355:ALA:HB1	1:F:521:ILE:HG12	1.98	0.45
1:F:584:GLN:HB3	1:F:598:THR:O	2.16	0.45
1:D:278:GLU:HG3	1:D:286:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:HD13	1:B:342:PRO:HD3	1.99	0.45
1:B:387:MET:O	1:B:387:MET:HG3	2.17	0.45
1:D:253:HIS:H	1:D:253:HIS:HD2	1.63	0.45
1:D:377:THR:CG2	1:D:378:LYS:N	2.79	0.45
1:D:588:LYS:HG3	1:D:637:ILE:HD11	1.99	0.45
1:F:193:ARG:CG	1:F:197:CYS:CB	2.94	0.45
1:A:212:VAL:CG2	1:A:299:TYR:CD1	3.00	0.45
1:B:138:LYS:HG3	1:B:138:LYS:H	1.56	0.45
1:E:262:ILE:HA	1:E:262:ILE:HD13	1.54	0.45
1:E:586:LEU:CD2	1:E:586:LEU:N	2.78	0.45
1:F:454:ILE:CG2	1:F:457:GLY:CA	2.91	0.45
1:D:406:ASP:CG	1:D:498:LEU:HD11	2.37	0.45
1:E:159:GLY:HA2	1:E:162:PHE:H	1.81	0.45
1:F:534:TRP:CH2	1:F:653:ASN:HB3	2.51	0.45
1:A:122:TYR:CE1	1:A:205:ASN:HB3	2.52	0.45
1:A:262:ILE:HD13	1:A:265:TRP:HZ3	1.82	0.45
1:B:641:ASP:HB2	6:B:809:HOH:O	2.15	0.45
1:D:459:SER:OG	1:D:462:LEU:HB2	2.17	0.45
1:E:191:ASP:OD1	1:E:193:ARG:HG2	2.16	0.45
1:E:455:TYR:O	1:E:455:TYR:CD1	2.70	0.45
1:F:196:GLU:HG3	6:F:837:HOH:O	2.16	0.45
1:F:264:LEU:CD2	1:F:264:LEU:O	2.65	0.45
1:F:495:ILE:HD12	1:F:495:ILE:HA	1.70	0.45
1:F:579:LEU:HB2	1:F:608:TRP:CD1	2.52	0.45
1:F:584:GLN:HG2	1:F:599:HIS:HA	1.99	0.45
1:B:113:LEU:HD12	1:B:504:ASP:HB3	1.98	0.44
1:C:286:ILE:HG22	1:C:290:LYS:HD2	1.98	0.44
1:C:197:CYS:SG	1:C:379:THR:HG23	2.57	0.44
1:D:172:GLU:HG2	1:D:251:LYS:NZ	2.32	0.44
1:D:650:GLU:HG3	1:D:652:ASN:HD21	1.81	0.44
1:E:154:LYS:HB3	1:E:154:LYS:HE3	1.90	0.44
1:E:404:LEU:CD2	1:E:404:LEU:N	2.73	0.44
1:A:400:PHE:O	1:A:403:GLY:CA	2.65	0.44
1:B:597:ILE:O	1:B:597:ILE:HG22	2.16	0.44
1:F:166:ILE:O	1:F:170:ILE:HG13	2.17	0.44
1:F:210:SER:OG	1:F:241:GLU:HG2	2.18	0.44
1:A:258:LEU:HD12	1:A:262:ILE:HG12	1.99	0.44
1:C:414:GLY:CA	1:C:415:GLU:CB	2.91	0.44
1:C:447:TRP:O	1:C:448:GLN:HG2	2.17	0.44
1:D:339:GLU:OE1	1:D:339:GLU:N	2.47	0.44
1:D:486:GLU:HA	1:D:534:TRP:CH2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:HG2	1:A:445:GLU:H	1.47	0.44
1:A:358:TRP:O	1:A:480:PHE:HA	2.17	0.44
1:C:377:THR:HG22	1:C:378:LYS:N	2.31	0.44
1:C:421:TYR:HB3	1:C:425:GLN:HE21	1.82	0.44
1:C:513:PHE:CE1	1:C:517:ILE:CD1	2.98	0.44
1:D:262:ILE:HD13	1:D:262:ILE:HA	1.78	0.44
1:D:214:VAL:HG12	4:D:702:UDP:H1'	1.99	0.44
1:F:207:LEU:CD1	1:F:319:SER:HA	2.47	0.44
1:A:122:TYR:CD1	1:A:205:ASN:HB3	2.52	0.44
1:A:513:PHE:CD1	1:A:517:ILE:HG12	2.52	0.44
1:B:410:GLN:N	1:B:464:ASN:HD21	2.15	0.44
1:B:627:ASP:OD1	1:B:646:THR:HB	2.18	0.44
1:C:375:ARG:HE	1:C:382:TYR:HB3	1.81	0.44
1:D:469:VAL:HG22	1:D:473:TRP:CD2	2.52	0.44
1:E:189:VAL:CG1	1:E:190:ASN:N	2.80	0.44
1:E:202:TYR:OH	1:E:313:PRO:HG3	2.18	0.44
1:F:172:GLU:HG3	1:F:251:LYS:NZ	2.32	0.44
1:F:311:TYR:CZ	1:F:315:VAL:HG21	2.53	0.44
1:A:363:LYS:HD2	1:A:525:TYR:OH	2.18	0.44
1:A:301:ASP:H	1:A:391:LEU:CD2	2.31	0.44
1:B:332:VAL:HG22	1:B:442:TYR:CE2	2.53	0.44
1:C:192:LEU:HD13	1:C:342:PRO:HD3	2.00	0.44
1:C:411:ILE:C	1:C:411:ILE:CD1	2.86	0.44
1:A:457:GLY:C	1:A:459:SER:CB	2.86	0.44
1:D:498:LEU:HA	1:D:498:LEU:HD23	1.75	0.44
1:E:264:LEU:HD22	1:E:264:LEU:O	2.17	0.44
1:E:312:ALA:HB3	1:E:313:PRO:HD3	1.99	0.44
1:A:138:LYS:H	1:A:138:LYS:HG3	1.59	0.44
1:B:172:GLU:CG	1:B:251:LYS:NZ	2.81	0.44
1:B:248:PHE:CE1	1:B:275:GLU:O	2.71	0.44
1:C:353:ARG:HG2	1:C:365:VAL:HG23	1.99	0.44
1:C:628:ARG:CG	1:C:628:ARG:NH1	2.75	0.44
1:D:211:VAL:HA	1:D:298:ILE:O	2.17	0.44
1:E:410:GLN:HB3	1:E:411:ILE:HD13	2.00	0.44
1:F:286:ILE:HG22	1:F:290:LYS:HD2	2.00	0.44
1:F:454:ILE:O	1:F:454:ILE:HG23	2.18	0.44
1:B:447:TRP:C	1:B:448:GLN:CG	2.86	0.44
1:B:495:ILE:HD12	1:B:495:ILE:HA	1.67	0.44
1:C:551:LYS:HG2	1:C:555:GLY:HA3	1.99	0.44
1:D:312:ALA:HB3	1:D:313:PRO:HD3	1.99	0.44
1:E:225:ARG:O	1:E:229:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:370:GLN:CD	1:F:370:GLN:H	2.21	0.44
1:F:326:THR:HG23	1:F:433:VAL:HG23	1.99	0.44
1:A:341:ILE:CG2	1:B:632:LEU:CB	2.85	0.43
1:B:539:GLY:HA3	1:B:628:ARG:NH2	2.33	0.43
1:C:421:TYR:HB3	1:C:425:GLN:NE2	2.33	0.43
1:C:455:TYR:N	1:C:455:TYR:CD1	2.86	0.43
1:D:373:ARG:CD	6:D:805:HOH:O	2.65	0.43
1:A:467:ARG:CZ	1:A:495:ILE:CD1	2.95	0.43
1:B:116:LYS:HB3	1:B:116:LYS:HE2	1.81	0.43
1:B:573:ILE:HA	1:B:578:GLN:O	2.18	0.43
1:C:368:THR:HB	1:C:370:GLN:OE1	2.18	0.43
1:D:458:SER:HB2	1:D:657:VAL:O	2.19	0.43
1:A:457:GLY:CA	1:A:459:SER:HB2	2.49	0.43
1:C:239:LEU:HD13	1:C:268:LEU:HD11	2.00	0.43
1:C:412:TRP:O	1:C:461:THR:CG2	2.54	0.43
1:D:211:VAL:CG2	1:D:242:ILE:HG12	2.46	0.43
1:F:548:SER:O	1:F:551:LYS:HB2	2.17	0.43
1:E:332:VAL:HG22	1:E:442:TYR:CE2	2.54	0.43
1:F:195:GLU:OE2	1:F:195:GLU:HA	2.18	0.43
1:B:574:ASN:ND2	1:B:578:GLN:OE1	2.51	0.43
1:B:632:LEU:HD11	1:B:634:GLN:HB2	1.95	0.43
1:C:312:ALA:N	1:C:313:PRO:CD	2.82	0.43
1:C:462:LEU:CD1	1:C:487:SER:CB	2.94	0.43
1:D:282:GLN:HG2	6:D:815:HOH:O	2.16	0.43
1:D:394:ILE:HD12	1:D:399:PHE:CG	2.53	0.43
1:D:410:GLN:HG3	6:D:844:HOH:O	2.18	0.43
1:D:458:SER:HB3	1:D:463:LYS:HZ2	1.84	0.43
1:E:136:GLU:CD	1:E:193:ARG:HH22	2.14	0.43
1:E:325:CYS:SG	1:E:394:ILE:HG23	2.59	0.43
1:E:548:SER:O	1:E:551:LYS:HB2	2.19	0.43
1:F:532:VAL:HB	1:F:573:ILE:HG23	2.01	0.43
1:A:191:ASP:OD1	1:A:193:ARG:CG	2.58	0.43
1:A:218:GLU:O	1:A:253:HIS:HE1	2.01	0.43
1:A:394:ILE:CD1	1:A:399:PHE:CG	3.01	0.43
1:A:586:LEU:CD2	1:A:586:LEU:N	2.81	0.43
1:C:254:LEU:O	1:C:273:ARG:NH2	2.52	0.43
1:C:346:GLY:HA3	1:C:366:PRO:CA	2.48	0.43
1:D:511:LYS:HB2	1:D:511:LYS:HE3	1.75	0.43
1:F:631:VAL:HG23	1:F:631:VAL:O	2.19	0.43
1:A:235:PRO:HB2	1:A:238:TYR:CD2	2.51	0.43
1:B:159:GLY:HA2	1:B:162:PHE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:GLU:HG2	1:B:519:TYR:OH	2.19	0.43
1:C:193:ARG:H	1:C:193:ARG:HG2	1.61	0.43
1:C:580:MET:HG2	1:C:585:CYS:SG	2.59	0.43
1:C:632:LEU:HD11	1:C:634:GLN:CB	2.40	0.43
1:D:218:GLU:HG3	1:D:302:ALA:CB	2.47	0.43
1:D:118:GLN:NE2	1:D:322:ARG:HG2	2.34	0.43
1:B:209:SER:OG	1:B:296:VAL:HG22	2.18	0.43
1:C:358:TRP:O	1:C:480:PHE:HA	2.19	0.43
1:C:539:GLY:HA3	1:C:628:ARG:NH2	2.33	0.43
1:D:153:ALA:HB2	1:D:190:ASN:CB	2.49	0.43
1:D:574:ASN:HB2	1:D:578:GLN:H	1.83	0.43
1:E:187:ARG:NH1	1:E:305:GLU:OE2	2.45	0.43
1:E:514:MET:CE	1:E:518:ALA:HB3	2.49	0.43
1:E:602:LEU:HA	1:E:602:LEU:HD23	1.71	0.43
1:F:276:ARG:HD2	1:F:278:GLU:OE2	2.19	0.43
1:F:365:VAL:HB	1:F:366:PRO:HD2	1.99	0.43
1:A:146:VAL:HA	1:A:147:GLY:HA2	1.63	0.43
1:A:411:ILE:HG23	1:A:412:TRP:H	1.84	0.43
1:B:574:ASN:HB3	1:B:576:ALA:H	1.84	0.43
1:C:616:ARG:HG2	1:C:618:THR:HG22	2.01	0.43
1:D:135:PHE:CZ	1:D:204:GLU:HG2	2.54	0.43
1:F:359:SER:HB2	1:F:484:ARG:NH1	2.34	0.43
1:F:411:ILE:HD13	1:F:460:PRO:HG2	2.00	0.43
1:A:447:TRP:O	1:A:448:GLN:HG2	2.19	0.43
1:B:484:ARG:NH2	6:B:803:HOH:O	2.50	0.43
1:C:454:ILE:O	1:C:458:SER:C	2.57	0.43
1:E:474:ASP:C	1:E:476:TYR:H	2.22	0.43
1:F:122:TYR:OH	1:F:206:LEU:HD21	2.19	0.43
1:F:453:PRO:HG3	1:F:455:TYR:OH	2.19	0.43
1:A:281:ILE:CD1	1:A:415:GLU:HG3	2.49	0.42
1:D:419:ILE:O	1:D:423:ILE:HG13	2.19	0.42
1:E:241:GLU:OE1	1:E:293:LEU:HD22	2.19	0.42
1:F:138:LYS:HG3	1:F:138:LYS:H	1.62	0.42
1:F:628:ARG:HG2	1:F:649:TRP:CH2	2.53	0.42
1:A:150:GLY:O	1:A:153:ALA:N	2.52	0.42
1:A:241:GLU:HA	1:A:268:LEU:HD22	2.00	0.42
1:A:301:ASP:OD2	1:A:303:HIS:NE2	2.52	0.42
1:A:513:PHE:HE1	1:A:517:ILE:HD11	1.82	0.42
1:B:136:GLU:OE1	1:B:193:ARG:NH2	2.52	0.42
1:C:264:LEU:O	1:C:264:LEU:HD22	2.19	0.42
1:C:193:ARG:NH1	1:C:308:VAL:CG2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:TYR:CE1	1:E:527:LEU:HG	2.54	0.42
1:E:534:TRP:O	1:E:653:ASN:ND2	2.49	0.42
1:A:326:THR:HG23	1:A:433:VAL:HG21	2.02	0.42
1:A:377:THR:HG22	1:A:378:LYS:N	2.34	0.42
1:A:488:GLN:NE2	6:A:815:HOH:O	2.50	0.42
1:A:540:PHE:CE2	1:A:541:GLU:HG3	2.54	0.42
1:B:414:GLY:CA	1:B:416:ASN:N	2.80	0.42
1:C:534:TRP:HA	1:C:651:MET:CE	2.49	0.42
1:D:239:LEU:HA	1:D:239:LEU:HD23	1.77	0.42
1:D:517:ILE:HG13	1:D:518:ALA:N	2.34	0.42
1:D:591:ASP:N	1:D:591:ASP:OD1	2.46	0.42
1:E:161:GLU:HG2	1:E:162:PHE:N	2.34	0.42
1:E:212:VAL:CG2	1:E:299:TYR:CE2	3.02	0.42
1:E:212:VAL:HG22	1:E:299:TYR:CD2	2.55	0.42
1:E:631:VAL:O	1:E:631:VAL:HG23	2.18	0.42
1:F:454:ILE:HG23	1:F:457:GLY:H	1.83	0.42
1:A:485:PRO:HB2	1:A:534:TRP:CD2	2.54	0.42
1:C:146:VAL:HA	1:C:147:GLY:HA2	1.57	0.42
1:C:603:ASN:O	1:C:606:LYS:HD2	2.18	0.42
1:D:132:LEU:HD22	1:D:132:LEU:N	2.34	0.42
1:D:160:PRO:CA	1:D:163:LYS:HG3	2.45	0.42
1:D:325:CYS:SG	1:D:394:ILE:HG23	2.60	0.42
1:E:262:ILE:CD1	1:E:265:TRP:HZ3	2.32	0.42
1:A:281:ILE:HD12	1:A:410:GLN:O	2.20	0.42
1:B:514:MET:HE1	1:B:518:ALA:CB	2.49	0.42
1:C:631:VAL:O	1:C:631:VAL:HG23	2.18	0.42
1:D:255:LYS:HG3	1:D:255:LYS:H	1.75	0.42
1:E:458:SER:HA	1:E:459:SER:HA	1.81	0.42
1:F:207:LEU:HD12	1:F:319:SER:OG	2.20	0.42
1:F:326:THR:HG23	1:F:433:VAL:HG21	2.01	0.42
1:F:454:ILE:HG23	1:F:457:GLY:C	2.40	0.42
1:C:138:LYS:HE3	1:C:138:LYS:HB2	1.86	0.42
1:E:231:ILE:HD12	1:E:265:TRP:CE2	2.55	0.42
1:A:276:ARG:CD	1:A:278:GLU:OE2	2.56	0.42
1:A:341:ILE:HG23	1:B:632:LEU:HA	2.00	0.42
1:A:455:TYR:O	1:A:455:TYR:HD1	2.03	0.42
1:B:403:GLY:HA2	1:B:404:LEU:HA	1.81	0.42
1:D:264:LEU:CD2	1:D:264:LEU:O	2.67	0.42
1:D:574:ASN:HB3	1:D:576:ALA:N	2.34	0.42
1:D:627:ASP:HB3	1:D:636:PHE:CD1	2.54	0.42
1:F:196:GLU:HB3	6:F:837:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ASN:HA	1:A:606:LYS:HD2	2.01	0.42
1:B:584:GLN:CG	1:B:598:THR:C	2.87	0.42
1:C:200:TRP:HE1	1:C:379:THR:CG2	2.33	0.42
1:C:532:VAL:HB	1:C:573:ILE:HG23	2.02	0.42
1:D:151:GLU:HA	1:D:152:LYS:C	2.40	0.42
1:E:326:THR:HG23	1:E:433:VAL:CG2	2.50	0.42
1:B:203:ASP:HB3	1:B:205:ASN:H	1.84	0.42
1:B:279:GLY:CA	1:B:411:ILE:HD12	2.50	0.42
1:C:379:THR:HG22	1:C:435:CYS:SG	2.47	0.42
1:C:548:SER:HA	1:C:557:VAL:HG23	2.02	0.42
1:D:534:TRP:O	1:D:653:ASN:ND2	2.51	0.42
1:D:546:ILE:CD1	1:D:626:LEU:HD21	2.49	0.42
1:E:326:THR:HG23	1:E:433:VAL:HG23	2.02	0.42
1:E:445:GLU:H	1:E:445:GLU:HG2	1.54	0.42
1:E:477:LYS:HG3	1:E:477:LYS:H	1.62	0.42
1:F:414:GLY:HA2	1:F:415:GLU:OE2	2.19	0.42
1:F:620:ILE:N	1:F:621:PRO:HD2	2.35	0.42
1:A:152:LYS:O	1:A:153:ALA:HB3	2.20	0.42
1:A:341:ILE:HG21	1:B:632:LEU:HB2	1.95	0.42
1:C:333:ILE:HB	1:C:441:ILE:HA	2.02	0.42
1:C:113:LEU:HB2	1:C:504:ASP:O	2.19	0.42
1:C:539:GLY:CA	1:C:628:ARG:NH2	2.82	0.42
1:D:253:HIS:N	1:D:253:HIS:CD2	2.85	0.42
1:E:576:ALA:O	1:E:577:ASN:HB2	2.20	0.42
1:F:403:GLY:HA2	1:F:404:LEU:HA	1.75	0.42
1:B:220:TRP:CZ3	1:B:257:LYS:HG2	2.54	0.41
1:D:170:ILE:O	1:D:174:GLY:N	2.47	0.41
1:D:172:GLU:CG	1:D:251:LYS:NZ	2.82	0.41
1:D:212:VAL:HG21	1:D:299:TYR:CE2	2.55	0.41
1:F:574:ASN:ND2	1:F:578:GLN:OE1	2.53	0.41
1:A:472:TRP:O	1:A:510:PHE:HB2	2.19	0.41
1:B:190:ASN:C	1:B:190:ASN:ND2	2.73	0.41
1:D:548:SER:HA	1:D:557:VAL:HG23	2.02	0.41
1:D:626:LEU:HD12	1:D:626:LEU:HA	1.91	0.41
1:F:211:VAL:O	1:F:211:VAL:CG2	2.67	0.41
1:B:143:PRO:HG2	1:B:146:VAL:HG22	2.03	0.41
1:B:553:ASN:HA	1:B:598:THR:HA	2.03	0.41
1:C:196:GLU:OE1	1:C:379:THR:CB	2.62	0.41
1:D:406:ASP:HB2	1:D:498:LEU:CD1	2.49	0.41
1:D:479:TYR:CD1	1:D:528:PRO:HD2	2.56	0.41
1:F:445:GLU:H	1:F:445:GLU:HG2	1.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PHE:O	1:A:403:GLY:N	2.54	0.41
1:E:187:ARG:O	1:E:187:ARG:HG3	2.20	0.41
1:E:211:VAL:HA	1:E:298:ILE:O	2.21	0.41
1:E:239:LEU:HD13	1:E:268:LEU:HD11	2.02	0.41
1:E:610:TYR:HB2	1:E:617:PHE:CE1	2.56	0.41
1:B:187:ARG:HD2	1:B:188:SER:O	2.20	0.41
1:B:513:PHE:CD1	1:B:517:ILE:HG12	2.55	0.41
1:B:539:GLY:CA	1:B:628:ARG:NH2	2.83	0.41
1:C:116:LYS:NZ	1:C:397:GLU:OE1	2.51	0.41
1:C:620:ILE:N	1:C:621:PRO:HD2	2.36	0.41
1:D:238:TYR:HB3	1:D:311:TYR:CE2	2.56	0.41
1:E:146:VAL:HA	1:E:147:GLY:HA2	1.61	0.41
1:E:632:LEU:HD13	1:E:633:HIS:N	2.34	0.41
1:F:520:ASP:O	1:F:523:SER:HB3	2.20	0.41
1:B:410:GLN:H	1:B:464:ASN:HD21	1.66	0.41
1:C:214:VAL:HG22	1:C:245:ILE:HB	2.03	0.41
1:C:565:MET:HE1	1:D:163:LYS:NZ	2.36	0.41
1:C:632:LEU:HA	1:D:341:ILE:HG23	2.03	0.41
1:D:176:ASN:C	1:D:176:ASN:ND2	2.74	0.41
1:E:211:VAL:CG2	1:E:242:ILE:HG12	2.50	0.41
1:B:406:ASP:HA	1:B:407:PRO:HD3	1.91	0.41
1:C:377:THR:HG22	1:C:379:THR:N	2.27	0.41
1:C:587:THR:OG1	1:C:588:LYS:N	2.51	0.41
1:D:153:ALA:HB2	1:D:190:ASN:H	1.85	0.41
1:D:306:VAL:CG2	1:D:310:TRP:CD2	3.04	0.41
1:F:454:ILE:CG2	1:F:457:GLY:HA3	2.51	0.41
1:B:278:GLU:HG3	1:B:286:ILE:CD1	2.51	0.41
1:B:463:LYS:O	1:B:467:ARG:HG3	2.21	0.41
1:C:419:ILE:HG13	1:C:423:ILE:HD11	2.01	0.41
1:E:190:ASN:C	1:E:190:ASN:ND2	2.73	0.41
1:A:300:LEU:HA	1:A:300:LEU:HD12	1.94	0.41
1:B:445:GLU:H	1:B:445:GLU:HG2	1.44	0.41
1:C:300:LEU:HD12	1:C:300:LEU:HA	1.92	0.41
1:C:332:VAL:O	1:C:340:ILE:HA	2.21	0.41
1:C:540:PHE:CD2	1:C:541:GLU:HG3	2.56	0.41
1:D:601:ASN:HB2	1:D:604:GLU:HG3	2.02	0.41
1:F:118:GLN:OE1	1:F:120:PHE:HB3	2.21	0.41
1:F:153:ALA:HB3	1:F:190:ASN:OD1	2.21	0.41
1:F:347:ASP:CB	1:F:351:TYR:O	2.65	0.41
1:F:553:ASN:HA	1:F:598:THR:HA	2.03	0.41
1:B:115:PHE:HE2	1:B:426:CYS:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD21	1:B:199:TYR:CE1	2.52	0.41
1:D:152:LYS:HD3	1:D:152:LYS:N	2.34	0.41
1:D:158:LEU:HD11	1:D:178:VAL:CG2	2.45	0.41
1:E:450:ASN:N	1:E:450:ASN:ND2	2.63	0.41
1:E:628:ARG:NH1	1:E:628:ARG:CG	2.82	0.41
1:F:632:LEU:HD11	1:F:634:GLN:CG	2.51	0.41
1:B:337:THR:O	1:B:338:TYR:HB2	2.19	0.41
1:C:118:GLN:NE2	1:C:321:ASP:HA	2.36	0.41
1:C:242:ILE:HB	1:C:269:VAL:HG22	2.02	0.41
1:D:122:TYR:OH	1:D:203:ASP:O	2.33	0.41
1:D:520:ASP:N	1:D:520:ASP:OD1	2.35	0.41
1:E:169:SER:HB2	1:E:177:MET:HB2	2.03	0.41
1:E:224:MET:HE3	1:E:227:VAL:HB	2.03	0.41
1:E:473:TRP:CZ3	1:E:480:PHE:HB2	2.56	0.41
1:F:347:ASP:O	1:F:350:GLY:N	2.41	0.41
1:F:385:PRO:HA	1:F:517:ILE:HD11	2.03	0.41
1:F:534:TRP:CZ2	1:F:653:ASN:HB3	2.56	0.41
1:A:312:ALA:N	1:A:313:PRO:HD2	2.36	0.40
1:B:371:GLU:OE2	1:B:383:ARG:NH2	2.53	0.40
1:B:601:ASN:HB2	1:B:604:GLU:OE1	2.21	0.40
1:C:341:ILE:HG23	1:D:631:VAL:O	2.21	0.40
1:C:450:ASN:N	1:C:450:ASN:ND2	2.62	0.40
1:E:380:GLU:HB2	1:E:381:PRO:HD2	2.02	0.40
1:F:422:LYS:HG2	1:F:472:TRP:HZ2	1.84	0.40
1:F:580:MET:HG2	1:F:585:CYS:SG	2.61	0.40
1:B:602:LEU:O	1:B:602:LEU:HD22	2.21	0.40
1:C:255:LYS:O	1:C:257:LYS:N	2.50	0.40
1:C:548:SER:O	1:C:551:LYS:HB2	2.21	0.40
1:E:162:PHE:O	1:E:166:ILE:HG13	2.21	0.40
1:E:242:ILE:HB	1:E:269:VAL:HG22	2.04	0.40
1:E:116:LYS:NZ	1:E:397:GLU:OE1	2.54	0.40
1:F:212:VAL:HG23	1:F:212:VAL:O	2.21	0.40
1:F:454:ILE:HG12	1:F:457:GLY:HA3	2.04	0.40
1:F:628:ARG:NH1	1:F:628:ARG:CG	2.84	0.40
1:A:131:ILE:O	1:A:199:TYR:HD1	2.05	0.40
1:A:346:GLY:HA3	1:A:366:PRO:CA	2.51	0.40
1:B:194:GLN:O	1:B:197:CYS:HB2	2.21	0.40
1:B:301:ASP:OD2	1:B:303:HIS:NE2	2.54	0.40
1:B:373:ARG:HD2	1:B:373:ARG:HA	1.90	0.40
1:B:200:TRP:CZ2	1:B:377:THR:HG21	2.55	0.40
1:B:484:ARG:NE	6:B:803:HOH:O	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLU:O	1:C:154:LYS:HB2	2.20	0.40
1:C:173:PHE:CD2	1:C:177:MET:HG3	2.55	0.40
1:D:149:PRO:HG2	1:D:182:MET:O	2.20	0.40
1:D:255:LYS:HA	1:D:273:ARG:NH2	2.36	0.40
1:E:204:GLU:N	1:E:204:GLU:OE1	2.51	0.40
1:E:286:ILE:HG22	1:E:290:LYS:HD2	2.04	0.40
1:F:132:LEU:O	1:F:201:HIS:CE1	2.74	0.40
1:F:411:ILE:CG2	1:F:412:TRP:H	2.25	0.40
1:F:412:TRP:O	1:F:461:THR:CG2	2.69	0.40
1:A:421:TYR:HB3	1:A:425:GLN:NE2	2.37	0.40
1:A:450:ASN:HD22	1:A:450:ASN:H	1.64	0.40
1:B:235:PRO:HB2	1:B:238:TYR:CD2	2.57	0.40
1:B:306:VAL:CG2	1:B:310:TRP:CD2	3.04	0.40
1:A:341:ILE:HG12	1:B:633:HIS:CD2	2.56	0.40
1:C:169:SER:HB2	1:C:177:MET:HB2	2.04	0.40
1:C:301:ASP:HB2	1:C:304:CYS:SG	2.61	0.40
1:D:255:LYS:O	1:D:256:GLU:HG2	2.21	0.40
1:D:207:LEU:HD11	1:D:319:SER:HA	2.04	0.40
1:D:537:ILE:HG21	1:D:546:ILE:HD12	2.03	0.40
1:E:301:ASP:OD2	1:E:440:HIS:NE2	2.39	0.40
1:F:641:ASP:C	1:F:641:ASP:OD1	2.59	0.40
1:A:349:ASP:OD2	1:A:378:LYS:HE3	2.21	0.40
1:A:300:LEU:HA	1:A:391:LEU:HD22	2.03	0.40
1:C:260:GLU:OE2	1:C:263:LYS:NZ	2.35	0.40
1:C:419:ILE:HA	1:C:419:ILE:HD12	1.93	0.40
1:D:122:TYR:OH	1:D:206:LEU:HD23	2.21	0.40
1:D:586:LEU:CD2	1:D:597:ILE:CG1	2.98	0.40
1:F:620:ILE:H	1:F:621:PRO:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	544/597 (91%)	516 (95%)	26 (5%)	2 (0%)	34 57
1	B	544/597 (91%)	520 (96%)	24 (4%)	0	100 100
1	C	544/597 (91%)	515 (95%)	27 (5%)	2 (0%)	34 57
1	D	534/597 (89%)	513 (96%)	20 (4%)	1 (0%)	47 71
1	E	544/597 (91%)	518 (95%)	26 (5%)	0	100 100
1	F	544/597 (91%)	509 (94%)	32 (6%)	3 (1%)	25 47
All	All	3254/3582 (91%)	3091 (95%)	155 (5%)	8 (0%)	47 71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	SER
1	F	411	ILE
1	F	413	GLY
1	D	176	ASN
1	C	453	PRO
1	C	460	PRO
1	F	453	PRO
1	A	592	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	480/525 (91%)	400 (83%)	80 (17%)	2 3
1	B	480/525 (91%)	395 (82%)	85 (18%)	2 3
1	C	480/525 (91%)	397 (83%)	83 (17%)	2 3
1	D	473/525 (90%)	418 (88%)	55 (12%)	5 10
1	E	480/525 (91%)	401 (84%)	79 (16%)	2 3
1	F	480/525 (91%)	406 (85%)	74 (15%)	2 4
All	All	2873/3150 (91%)	2417 (84%)	456 (16%)	2 4

All (456) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	127	LEU
1	A	132	LEU
1	A	138	LYS
1	A	139	GLU
1	A	151	GLU
1	A	152	LYS
1	A	154	LYS
1	A	156	LEU
1	A	164	GLN
1	A	176	ASN
1	A	178	VAL
1	A	182	MET
1	A	189	VAL
1	A	190	ASN
1	A	193	ARG
1	A	207	LEU
1	A	212	VAL
1	A	229	SER
1	A	239	LEU
1	A	250	ASN
1	A	255	LYS
1	A	258	LEU
1	A	262	ILE
1	A	264	LEU
1	A	268	LEU
1	A	270	LYS
1	A	276	ARG
1	A	277	ARG
1	A	293	LEU
1	A	296	VAL
1	A	300	LEU
1	A	301	ASP
1	A	306	VAL
1	A	308	VAL
1	A	320	LYS
1	A	326	THR
1	A	353	ARG
1	A	379	THR
1	A	394	ILE
1	A	395	GLU
1	A	402	LEU

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Mol	Chain	Res	Type
1	A	405	TYR
1	A	409	LEU
1	A	410	GLN
1	A	411	ILE
1	A	415	GLU
1	A	430	LEU
1	A	443	ARG
1	A	445	GLU
1	A	448	GLN
1	A	450	ASN
1	A	454	ILE
1	A	455	TYR
1	A	471	VAL
1	A	490	LEU
1	A	498	LEU
1	A	506	ASN
1	A	517	ILE
1	A	523	SER
1	A	527	LEU
1	A	547	ASP
1	A	551	LYS
1	A	557	VAL
1	A	572	ARG
1	A	579	LEU
1	A	586	LEU
1	A	588	LYS
1	A	591	ASP
1	A	597	ILE
1	A	598	THR
1	A	602	LEU
1	A	614	LEU
1	A	618	THR
1	A	633	HIS
1	A	634	GLN
1	A	642	SER
1	A	650	GLU
1	A	655	HIS
1	A	656	SER
1	B	114	THR
1	B	116	LYS
1	B	121	THR
1	B	127	LEU

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Mol	Chain	Res	Type
1	B	132	LEU
1	B	138	LYS
1	B	139	GLU
1	B	151	GLU
1	B	152	LYS
1	B	154	LYS
1	B	156	LEU
1	B	164	GLN
1	B	176	ASN
1	B	182	MET
1	B	187	ARG
1	B	190	ASN
1	B	193	ARG
1	B	198	LYS
1	B	203	ASP
1	B	211	VAL
1	B	212	VAL
1	B	229	SER
1	B	231	ILE
1	B	239	LEU
1	B	250	ASN
1	B	251	LYS
1	B	255	LYS
1	B	264	LEU
1	B	268	LEU
1	B	270	LYS
1	B	273	ARG
1	B	276	ARG
1	B	293	LEU
1	B	296	VAL
1	B	300	LEU
1	B	301	ASP
1	B	306	VAL
1	B	308	VAL
1	B	320	LYS
1	B	326	THR
1	B	349	ASP
1	B	353	ARG
1	B	359	SER
1	B	391	LEU
1	B	394	ILE
1	B	397	GLU

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Mol	Chain	Res	Type
1	B	406	ASP
1	B	409	LEU
1	B	411	ILE
1	B	415	GLU
1	B	430	LEU
1	B	443	ARG
1	B	445	GLU
1	B	448	GLN
1	B	450	ASN
1	B	455	TYR
1	B	456	VAL
1	B	461	THR
1	B	462	LEU
1	B	495	ILE
1	B	498	LEU
1	B	499	LYS
1	B	506	ASN
1	B	517	ILE
1	B	527	LEU
1	B	547	ASP
1	B	551	LYS
1	B	557	VAL
1	B	579	LEU
1	B	584	GLN
1	B	586	LEU
1	B	588	LYS
1	B	591	ASP
1	B	597	ILE
1	B	598	THR
1	B	600	CYS
1	B	602	LEU
1	B	614	LEU
1	B	618	THR
1	B	628	ARG
1	B	632	LEU
1	B	642	SER
1	B	650	GLU
1	B	655	HIS
1	B	656	SER
1	C	114	THR
1	C	116	LYS
1	C	127	LEU

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Mol	Chain	Res	Type
1	C	132	LEU
1	C	138	LYS
1	C	139	GLU
1	C	151	GLU
1	C	154	LYS
1	C	156	LEU
1	C	163	LYS
1	C	164	GLN
1	C	176	ASN
1	C	182	MET
1	C	189	VAL
1	C	190	ASN
1	C	193	ARG
1	C	194	GLN
1	C	204	GLU
1	C	211	VAL
1	C	212	VAL
1	C	229	SER
1	C	239	LEU
1	C	249	SER
1	C	250	ASN
1	C	252	GLU
1	C	255	LYS
1	C	264	LEU
1	C	270	LYS
1	C	276	ARG
1	C	277	ARG
1	C	293	LEU
1	C	300	LEU
1	C	301	ASP
1	C	306	VAL
1	C	308	VAL
1	C	320	LYS
1	C	326	THR
1	C	341	ILE
1	C	349	ASP
1	C	391	LEU
1	C	394	ILE
1	C	395	GLU
1	C	397	GLU
1	C	399	PHE
1	C	404	LEU

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Mol	Chain	Res	Type
1	C	409	LEU
1	C	410	GLN
1	C	415	GLU
1	C	430	LEU
1	C	443	ARG
1	C	445	GLU
1	C	448	GLN
1	C	450	ASN
1	C	455	TYR
1	C	459	SER
1	C	461	THR
1	C	462	LEU
1	C	498	LEU
1	C	506	ASN
1	C	517	ILE
1	C	523	SER
1	C	527	LEU
1	C	547	ASP
1	C	551	LYS
1	C	557	VAL
1	C	579	LEU
1	C	586	LEU
1	C	588	LYS
1	C	591	ASP
1	C	597	ILE
1	C	598	THR
1	C	600	CYS
1	C	602	LEU
1	C	613	ASN
1	C	614	LEU
1	C	618	THR
1	C	628	ARG
1	C	629	SER
1	C	632	LEU
1	C	646	THR
1	C	648	LYS
1	C	655	HIS
1	C	656	SER
1	D	116	LYS
1	D	134	ASN
1	D	152	LYS
1	D	176	ASN

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Mol	Chain	Res	Type
1	D	178	VAL
1	D	190	ASN
1	D	193	ARG
1	D	229	SER
1	D	231	ILE
1	D	237	LYS
1	D	239	LEU
1	D	249	SER
1	D	250	ASN
1	D	254	LEU
1	D	255	LYS
1	D	256	GLU
1	D	258	LEU
1	D	264	LEU
1	D	276	ARG
1	D	280	LEU
1	D	293	LEU
1	D	300	LEU
1	D	301	ASP
1	D	306	VAL
1	D	308	VAL
1	D	320	LYS
1	D	349	ASP
1	D	353	ARG
1	D	359	SER
1	D	394	ILE
1	D	397	GLU
1	D	402	LEU
1	D	406	ASP
1	D	409	LEU
1	D	411	ILE
1	D	430	LEU
1	D	462	LEU
1	D	471	VAL
1	D	490	LEU
1	D	517	ILE
1	D	523	SER
1	D	527	LEU
1	D	542	THR
1	D	551	LYS
1	D	557	VAL
1	D	579	LEU

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Mol	Chain	Res	Type
1	D	584	GLN
1	D	597	ILE
1	D	600	CYS
1	D	602	LEU
1	D	614	LEU
1	D	628	ARG
1	D	631	VAL
1	D	633	HIS
1	D	656	SER
1	E	127	LEU
1	E	132	LEU
1	E	139	GLU
1	E	151	GLU
1	E	152	LYS
1	E	154	LYS
1	E	155	PRO
1	E	156	LEU
1	E	164	GLN
1	E	176	ASN
1	E	182	MET
1	E	190	ASN
1	E	193	ARG
1	E	211	VAL
1	E	212	VAL
1	E	229	SER
1	E	239	LEU
1	E	251	LYS
1	E	255	LYS
1	E	262	ILE
1	E	264	LEU
1	E	268	LEU
1	E	273	ARG
1	E	276	ARG
1	E	277	ARG
1	E	293	LEU
1	E	300	LEU
1	E	301	ASP
1	E	306	VAL
1	E	320	LYS
1	E	341	ILE
1	E	379	THR
1	E	391	LEU

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Mol	Chain	Res	Type
1	E	394	ILE
1	E	395	GLU
1	E	404	LEU
1	E	405	TYR
1	E	411	ILE
1	E	415	GLU
1	E	418	GLU
1	E	430	LEU
1	E	443	ARG
1	E	445	GLU
1	E	448	GLN
1	E	450	ASN
1	E	454	ILE
1	E	456	VAL
1	E	459	SER
1	E	461	THR
1	E	475	GLU
1	E	477	LYS
1	E	498	LEU
1	E	499	LYS
1	E	506	ASN
1	E	517	ILE
1	E	523	SER
1	E	527	LEU
1	E	542	THR
1	E	547	ASP
1	E	551	LYS
1	E	557	VAL
1	E	579	LEU
1	E	586	LEU
1	E	588	LYS
1	E	591	ASP
1	E	597	ILE
1	E	598	THR
1	E	600	CYS
1	E	602	LEU
1	E	604	GLU
1	E	614	LEU
1	E	618	THR
1	E	628	ARG
1	E	632	LEU
1	E	638	SER

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Mol	Chain	Res	Type
1	E	645	THR
1	E	646	THR
1	E	655	HIS
1	E	656	SER
1	F	114	THR
1	F	116	LYS
1	F	127	LEU
1	F	132	LEU
1	F	139	GLU
1	F	146	VAL
1	F	151	GLU
1	F	154	LYS
1	F	156	LEU
1	F	163	LYS
1	F	164	GLN
1	F	176	ASN
1	F	178	VAL
1	F	190	ASN
1	F	229	SER
1	F	231	ILE
1	F	237	LYS
1	F	239	LEU
1	F	249	SER
1	F	250	ASN
1	F	255	LYS
1	F	264	LEU
1	F	270	LYS
1	F	276	ARG
1	F	277	ARG
1	F	293	LEU
1	F	300	LEU
1	F	301	ASP
1	F	306	VAL
1	F	320	LYS
1	F	353	ARG
1	F	379	THR
1	F	391	LEU
1	F	394	ILE
1	F	397	GLU
1	F	404	LEU
1	F	415	GLU
1	F	430	LEU

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Mol	Chain	Res	Type
1	F	443	ARG
1	F	445	GLU
1	F	448	GLN
1	F	450	ASN
1	F	454	ILE
1	F	461	THR
1	F	462	LEU
1	F	471	VAL
1	F	498	LEU
1	F	499	LYS
1	F	506	ASN
1	F	517	ILE
1	F	520	ASP
1	F	527	LEU
1	F	542	THR
1	F	547	ASP
1	F	551	LYS
1	F	557	VAL
1	F	579	LEU
1	F	586	LEU
1	F	588	LYS
1	F	591	ASP
1	F	597	ILE
1	F	598	THR
1	F	600	CYS
1	F	602	LEU
1	F	618	THR
1	F	620	ILE
1	F	628	ARG
1	F	632	LEU
1	F	645	THR
1	F	646	THR
1	F	648	LYS
1	F	651	MET
1	F	655	HIS
1	F	656	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	176	ASN

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Mol	Chain	Res	Type
1	A	190	ASN
1	A	194	GLN
1	A	201	HIS
1	A	253	HIS
1	A	266	ASN
1	A	425	GLN
1	A	450	ASN
1	A	568	ASN
1	A	574	ASN
1	A	578	GLN
1	A	603	ASN
1	A	647	GLN
1	A	653	ASN
1	B	118	GLN
1	B	176	ASN
1	B	190	ASN
1	B	201	HIS
1	B	253	HIS
1	B	343	GLN
1	B	425	GLN
1	B	450	ASN
1	B	568	ASN
1	B	574	ASN
1	B	578	GLN
1	B	603	ASN
1	B	647	GLN
1	B	653	ASN
1	C	118	GLN
1	C	176	ASN
1	C	190	ASN
1	C	253	HIS
1	C	266	ASN
1	C	343	GLN
1	C	410	GLN
1	C	425	GLN
1	C	450	ASN
1	C	574	ASN
1	C	578	GLN
1	C	599	HIS
1	C	603	ASN
1	C	647	GLN
1	C	653	ASN

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Mol	Chain	Res	Type
1	D	118	GLN
1	D	176	ASN
1	D	201	HIS
1	D	266	ASN
1	D	410	GLN
1	D	425	GLN
1	D	506	ASN
1	D	568	ASN
1	D	574	ASN
1	D	578	GLN
1	D	599	HIS
1	D	603	ASN
1	D	613	ASN
1	D	647	GLN
1	D	652	ASN
1	D	655	HIS
1	E	118	GLN
1	E	176	ASN
1	E	190	ASN
1	E	253	HIS
1	E	425	GLN
1	E	450	ASN
1	E	464	ASN
1	E	568	ASN
1	E	574	ASN
1	E	578	GLN
1	E	599	HIS
1	E	603	ASN
1	E	647	GLN
1	E	653	ASN
1	F	118	GLN
1	F	176	ASN
1	F	190	ASN
1	F	201	HIS
1	F	425	GLN
1	F	450	ASN
1	F	464	ASN
1	F	568	ASN
1	F	574	ASN
1	F	578	GLN
1	F	599	HIS
1	F	603	ASN

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Mol	Chain	Res	Type
1	F	647	GLN
1	F	653	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	D	701	-	15,15,15	1.56	2 (13%)	21,21,21	1.04	1 (4%)
4	UDP	D	702	2	20,26,26	1.69	4 (20%)	25,40,40	1.47	2 (8%)
5	UD2	D	704	-	34,41,41	3.85	19 (55%)	45,62,62	2.56	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	701	-	-	1/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UDP	D	702	2	-	7/14/32/32	0/2/2/2
5	UD2	D	704	-	-	2/24/63/63	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	704	UD2	PB-O1'	10.34	1.87	1.60
5	D	704	UD2	C6-N1	8.94	1.46	1.35
5	D	704	UD2	C4-N3	8.18	1.47	1.33
5	D	704	UD2	O4B-C1B	6.92	1.50	1.41
5	D	704	UD2	O4B-C4B	5.90	1.58	1.45
5	D	704	UD2	O5'-C1'	4.78	1.54	1.41
5	D	704	UD2	C2-N3	4.65	1.47	1.38
4	D	702	UDP	C4-N3	4.61	1.41	1.33
3	D	701	NAG	O5-C1	4.60	1.54	1.42
5	D	704	UD2	O3B-C3B	3.72	1.51	1.43
5	D	704	UD2	O4'-C4'	3.34	1.50	1.43
5	D	704	UD2	C2B-C1B	3.33	1.58	1.53
5	D	704	UD2	C3'-C2'	3.17	1.59	1.53
4	D	702	UDP	PB-O2B	3.12	1.66	1.54
5	D	704	UD2	O2'-C2B	3.06	1.50	1.43
5	D	704	UD2	O3'-C3'	3.00	1.50	1.43
5	D	704	UD2	O5'-C5'	2.98	1.51	1.44
5	D	704	UD2	PA-O5B	2.95	1.71	1.59
5	D	704	UD2	C8'-C7'	2.87	1.56	1.50
4	D	702	UDP	PB-O1B	2.61	1.59	1.50
5	D	704	UD2	C2'-N2'	2.61	1.50	1.45
4	D	702	UDP	C6-N1	2.38	1.38	1.35
5	D	704	UD2	C3B-C2B	2.34	1.59	1.53
5	D	704	UD2	PA-O2A	2.26	1.58	1.50
3	D	701	NAG	C3-C2	2.16	1.57	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	704	UD2	O3A-PB-O1'	-8.79	84.76	102.48
5	D	704	UD2	O1'-PB-O2B	-7.91	79.79	109.47
5	D	704	UD2	O4B-C1B-C2B	-6.38	97.60	106.93
5	D	704	UD2	PB-O3A-PA	-6.05	112.08	132.83
4	D	702	UDP	PA-O3A-PB	-5.25	114.81	132.83
5	D	704	UD2	O1B-PB-O1'	-4.31	89.79	106.78
4	D	702	UDP	C5-C4-N3	-4.06	114.38	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	704	UD2	O1B-PB-O2B	2.84	126.30	112.24
3	D	701	NAG	C1-O5-C5	-2.53	108.88	113.66
5	D	704	UD2	C1'-O5'-C5'	-2.39	108.99	113.69
5	D	704	UD2	O5'-C1'-O1'	-2.31	108.34	111.36
5	D	704	UD2	O5B-PA-O2A	2.00	116.89	109.07

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	704	UD2	C5B-O5B-PA-O3A
4	D	702	UDP	C2'-C1'-N1-C6
4	D	702	UDP	O4'-C1'-N1-C6
4	D	702	UDP	C5'-O5'-PA-O1A
3	D	701	NAG	O5-C5-C6-O6
4	D	702	UDP	C5'-O5'-PA-O3A
5	D	704	UD2	C5B-O5B-PA-O2A
4	D	702	UDP	C5'-O5'-PA-O2A
4	D	702	UDP	O4'-C4'-C5'-O5'
4	D	702	UDP	PB-O3A-PA-O2A

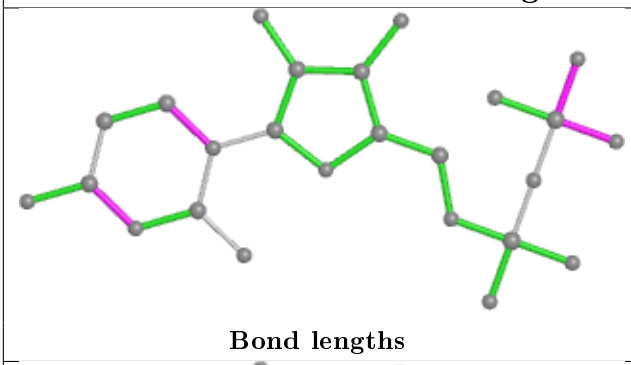
There are no ring outliers.

3 monomers are involved in 6 short contacts:

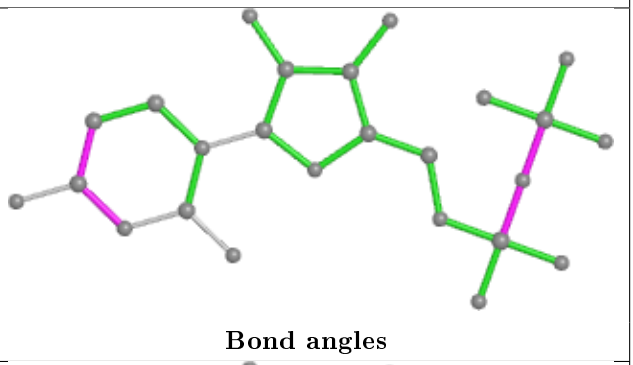
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	NAG	1	0
4	D	702	UDP	2	0
5	D	704	UD2	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

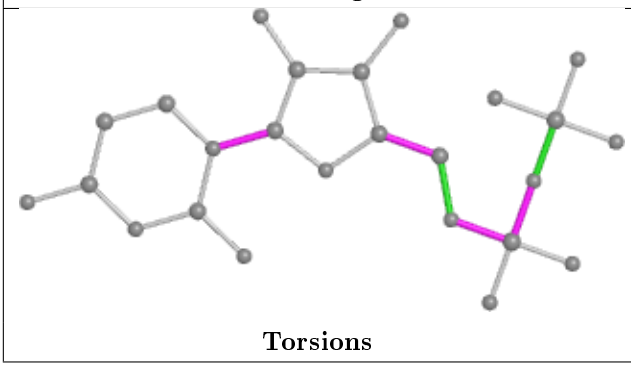
Ligand UDP D 702



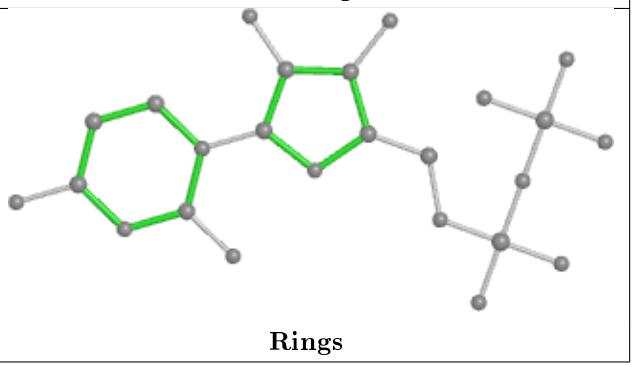
Bond lengths



Bond angles

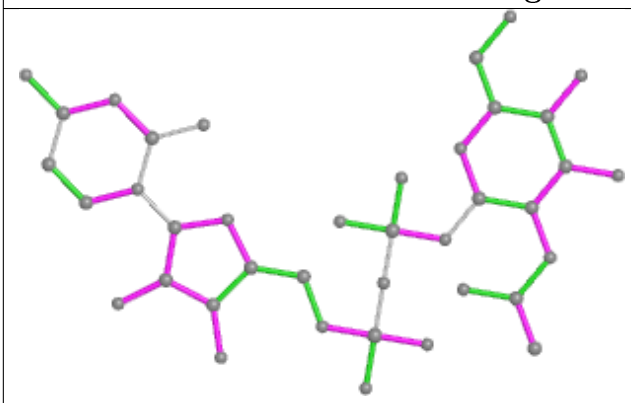


Torsions

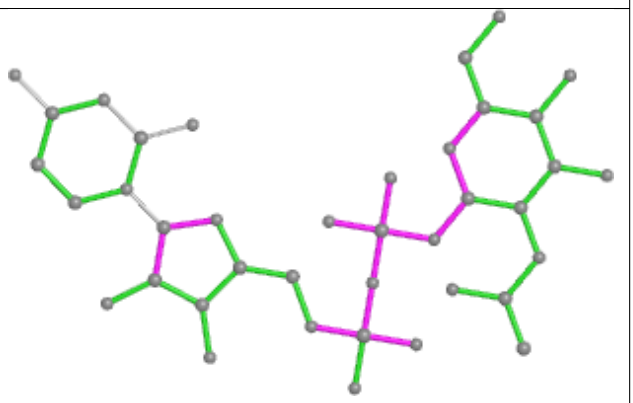


Rings

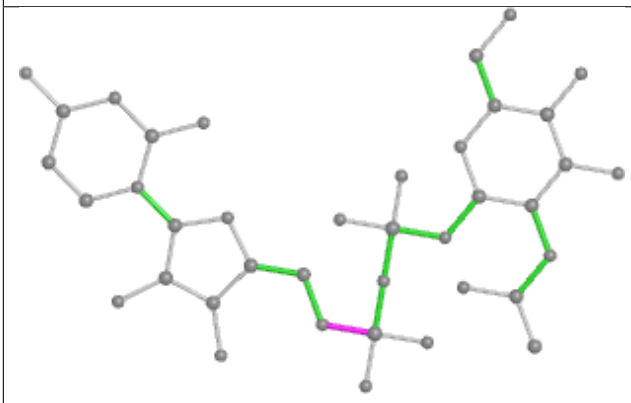
Ligand UD2 D 704



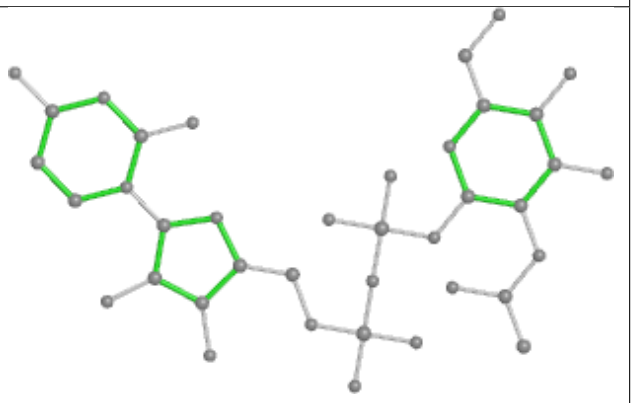
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	546/597 (91%)	-0.10	15 (2%)	54	48	23, 33, 59, 111	0
1	B	546/597 (91%)	-0.00	14 (2%)	56	50	26, 37, 64, 116	0
1	C	546/597 (91%)	0.22	27 (4%)	29	23	24, 42, 82, 138	0
1	D	538/597 (90%)	0.07	11 (2%)	65	60	29, 47, 75, 92	0
1	E	546/597 (91%)	0.19	32 (5%)	22	17	26, 46, 83, 154	0
1	F	546/597 (91%)	0.46	42 (7%)	13	10	34, 59, 86, 136	0
All	All	3268/3582 (91%)	0.14	141 (4%)	35	28	23, 43, 79, 154	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	SER	14.3
1	F	455	TYR	11.4
1	C	454	ILE	10.7
1	E	657	VAL	10.0
1	C	456	VAL	9.8
1	C	657	VAL	8.7
1	C	458	SER	8.5
1	E	452	PRO	8.5
1	F	450	ASN	8.3
1	F	452	PRO	8.0
1	A	457	GLY	7.8
1	F	451	PRO	7.4
1	C	455	TYR	7.4
1	E	456	VAL	6.9
1	B	457	GLY	6.7
1	A	452	PRO	6.5
1	B	458	SER	6.5
1	C	452	PRO	6.4
1	E	457	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	456	VAL	5.6
1	E	455	TYR	5.5
1	E	458	SER	5.5
1	C	450	ASN	5.5
1	A	451	PRO	5.3
1	C	457	GLY	5.0
1	F	446	GLY	5.0
1	F	448	GLN	4.9
1	C	453	PRO	4.9
1	B	452	PRO	4.9
1	C	451	PRO	4.8
1	F	456	VAL	4.8
1	E	453	PRO	4.7
1	A	454	ILE	4.7
1	F	147	GLY	4.6
1	A	453	PRO	4.4
1	E	454	ILE	4.3
1	B	453	PRO	4.3
1	E	591	ASP	4.3
1	B	451	PRO	4.2
1	B	112	TYR	4.2
1	E	449	GLY	4.2
1	E	593	SER	4.2
1	F	120	PHE	4.1
1	F	112	TYR	4.0
1	E	451	PRO	4.0
1	E	656	SER	4.0
1	F	453	PRO	3.8
1	C	112	TYR	3.8
1	B	455	TYR	3.8
1	B	450	ASN	3.7
1	A	455	TYR	3.6
1	C	591	ASP	3.6
1	F	454	ILE	3.6
1	B	454	ILE	3.5
1	F	162	PHE	3.4
1	E	605	PHE	3.4
1	E	602	LEU	3.4
1	F	121	THR	3.4
1	E	556	PHE	3.4
1	E	655	HIS	3.3
1	E	450	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	459	SER	3.2
1	B	346	GLY	3.1
1	C	599	HIS	3.1
1	E	643	SER	3.1
1	F	152	LYS	3.0
1	F	449	GLY	3.0
1	F	591	ASP	3.0
1	A	403	GLY	3.0
1	D	448	GLN	2.9
1	C	373	ARG	2.9
1	C	147	GLY	2.9
1	E	590	ALA	2.8
1	F	179	ALA	2.8
1	F	256	GLU	2.8
1	A	112	TYR	2.8
1	F	132	LEU	2.8
1	E	346	GLY	2.8
1	D	252	GLU	2.7
1	C	644	LYS	2.7
1	D	139	GLU	2.7
1	F	172	GLU	2.7
1	C	605	PHE	2.7
1	C	638	SER	2.7
1	D	138	LYS	2.6
1	D	254	LEU	2.6
1	F	376	LYS	2.5
1	A	450	ASN	2.5
1	F	447	TRP	2.5
1	F	632	LEU	2.5
1	C	540	PHE	2.5
1	F	346	GLY	2.5
1	E	588	LYS	2.5
1	F	131	ILE	2.5
1	F	588	LYS	2.5
1	F	164	GLN	2.4
1	F	127	LEU	2.4
1	C	593	SER	2.4
1	E	603	ASN	2.4
1	C	643	SER	2.4
1	E	489	ALA	2.4
1	E	147	GLY	2.4
1	F	138	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	145	VAL	2.4
1	A	591	ASP	2.3
1	F	266	ASN	2.3
1	F	126	VAL	2.3
1	F	178	VAL	2.3
1	F	590	ALA	2.3
1	B	456	VAL	2.3
1	A	147	GLY	2.3
1	F	196	GLU	2.3
1	E	638	SER	2.3
1	E	448	GLN	2.3
1	D	248	PHE	2.3
1	A	449	GLY	2.3
1	F	611	PHE	2.3
1	F	159	GLY	2.2
1	C	656	SER	2.2
1	B	147	GLY	2.2
1	E	490	LEU	2.2
1	F	255	LYS	2.2
1	C	640	CYS	2.2
1	D	266	ASN	2.2
1	E	601	ASN	2.2
1	D	119	THR	2.2
1	E	589	GLY	2.2
1	E	112	TYR	2.2
1	B	632	LEU	2.2
1	C	604	GLU	2.2
1	F	637	ILE	2.1
1	D	132	LEU	2.1
1	A	657	VAL	2.1
1	D	112	TYR	2.1
1	B	449	GLY	2.1
1	E	348	GLU	2.1
1	F	275	GLU	2.1
1	D	377	THR	2.1
1	C	617	PHE	2.0
1	C	616	ARG	2.0
1	F	626	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

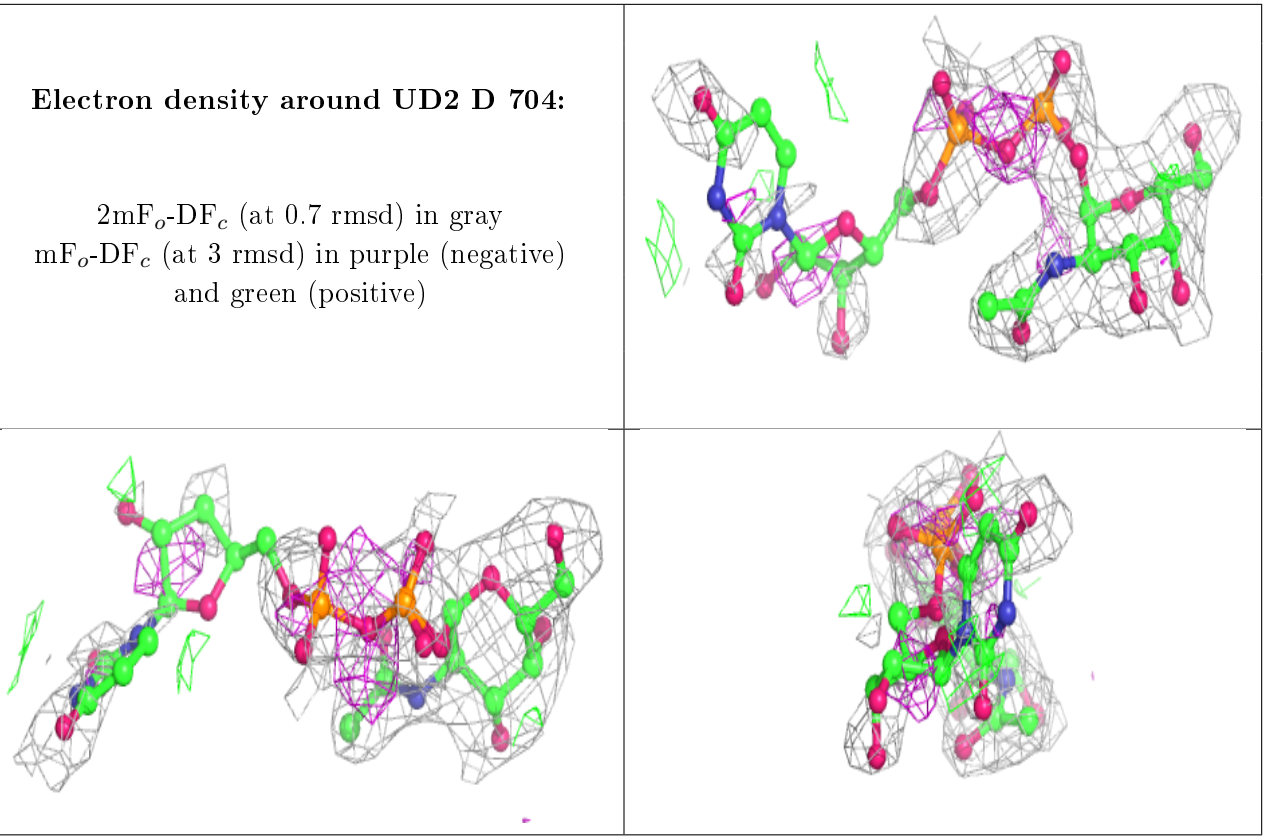
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	A	701	1/1	0.22	0.32	100,100,100,100	0
2	MN	F	701	1/1	0.66	0.32	91,91,91,91	0
2	MN	C	701	1/1	0.70	0.27	93,93,93,93	0
2	MN	E	701	1/1	0.78	0.19	82,82,82,82	0
3	NAG	D	701	15/15	0.83	0.33	52,68,79,82	0
5	UD2	D	704	39/39	0.85	0.33	36,81,113,113	0
2	MN	B	701	1/1	0.85	0.22	87,87,87,87	0
4	UDP	D	702	25/25	0.86	0.28	55,69,81,82	0
2	MN	D	703	1/1	0.97	0.14	56,56,56,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

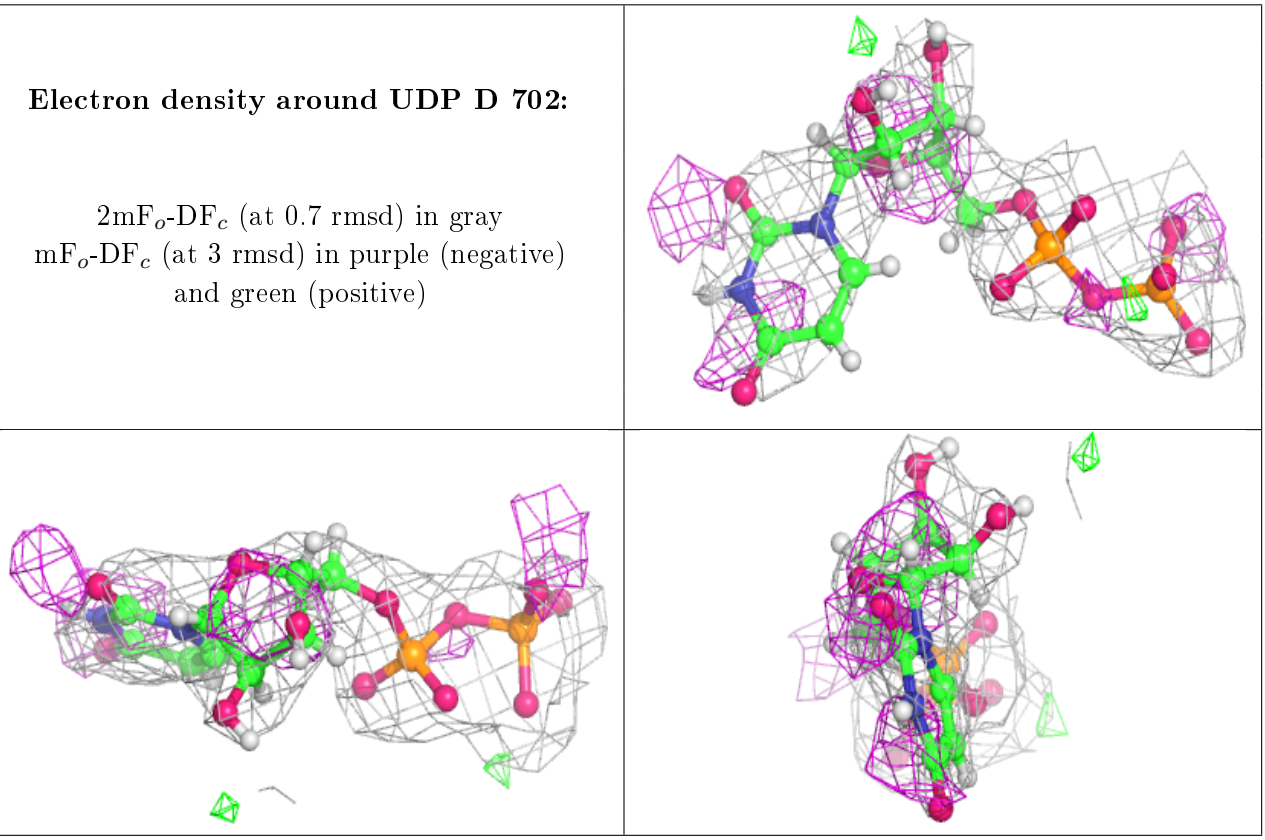
Electron density around UD2 D 704:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around UDP D 702:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.